Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2025 – 07:55 PM JST

PDB ID	:	8X78
Title	:	Crystal Structure of N-Acyl Homoserine Lactone Lactonase from Pseudomonas poae
Authors	:	Li, X.H.; Su, D.
Deposited on	:	2023-11-23
Resolution	:	2.36 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:

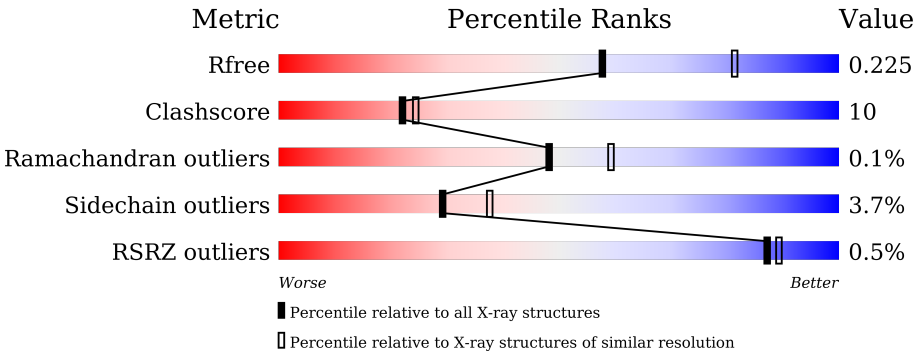
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.36 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	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	80% 14% • 6%
1	B	306	79% 14% • 6%
1	C	306	76% 17% • 6%
1	D	306	78% 15% • 6%
1	E	306	78% 15% • 6%
1	F	306	80% 15% 5%

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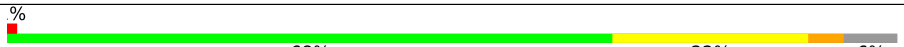
Mol	Chain	Length	Quality of chain
1	G	306	
1	H	306	
1	I	306	
1	J	306	
1	K	306	
1	L	306	

2 Entry composition (i)

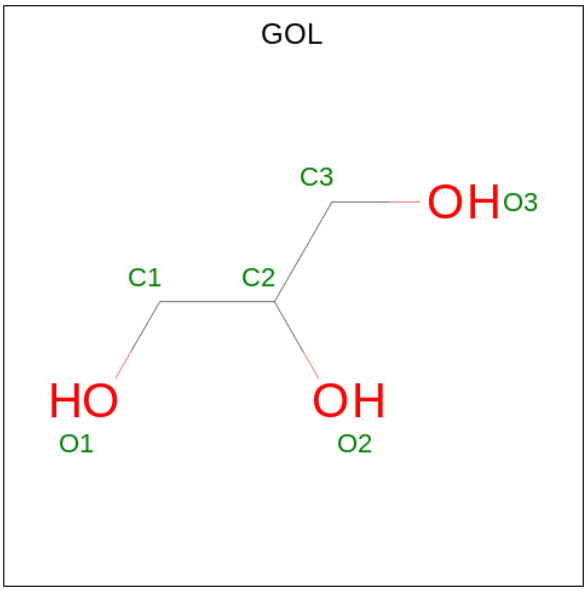
There are 4 unique types of molecules in this entry. The entry contains 28301 atoms, of which 104 are hydrogens and 0 are deuteriums.

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 Glyoxylase, beta-lactamase superfamily II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	287	Total	C	N	O	S	0	0	0
			2310	1467	399	434	10			
1	K	287	Total	C	N	O	S	0	0	0
			2306	1466	396	434	10			
1	G	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			
1	H	286	Total	C	N	O	S	0	0	0
			2298	1461	395	432	10			
1	I	285	Total	C	N	O	S	0	0	0
			2288	1455	391	432	10			
1	J	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			
1	F	291	Total	C	N	O	S	0	0	0
			2338	1483	403	442	10			
1	E	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			
1	A	289	Total	C	N	O	S	0	0	0
			2324	1477	401	436	10			
1	B	288	Total	C	N	O	S	0	0	0
			2314	1470	397	437	10			
1	C	287	Total	C	N	O	S	0	0	0
			2310	1467	399	434	10			
1	D	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	H	O	0	0
			14	3	8	3		
2	K	1	Total	C	H	O	0	0
			14	3	8	3		
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	H	1	Total	C	H	O	0	0
			14	3	8	3		
2	I	1	Total	C	H	O	0	0
			14	3	8	3		
2	J	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Inter-

est" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	13	Total O 13 13	0	0
4	K	5	Total O 5 5	0	0
4	G	4	Total O 4 4	0	0
4	H	8	Total O 8 8	0	0
4	I	14	Total O 14 14	0	0
4	J	34	Total O 34 34	0	0
4	F	37	Total O 37 37	0	0

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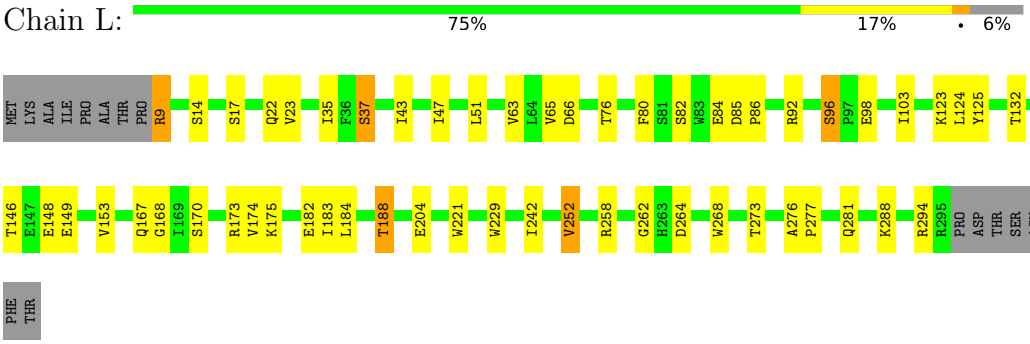
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	33	Total O 33 33	0	0
4	A	56	Total O 56 56	0	0
4	B	61	Total O 61 61	0	0
4	C	37	Total O 37 37	0	0
4	D	37	Total O 37 37	0	0

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.

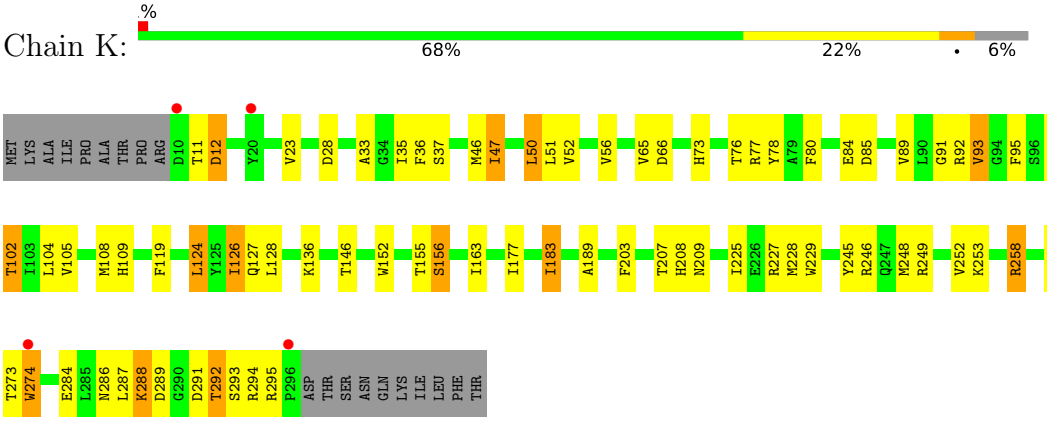
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain L:



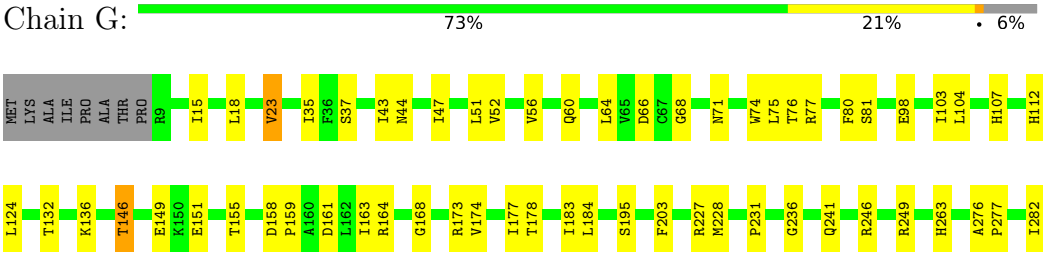
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain K:



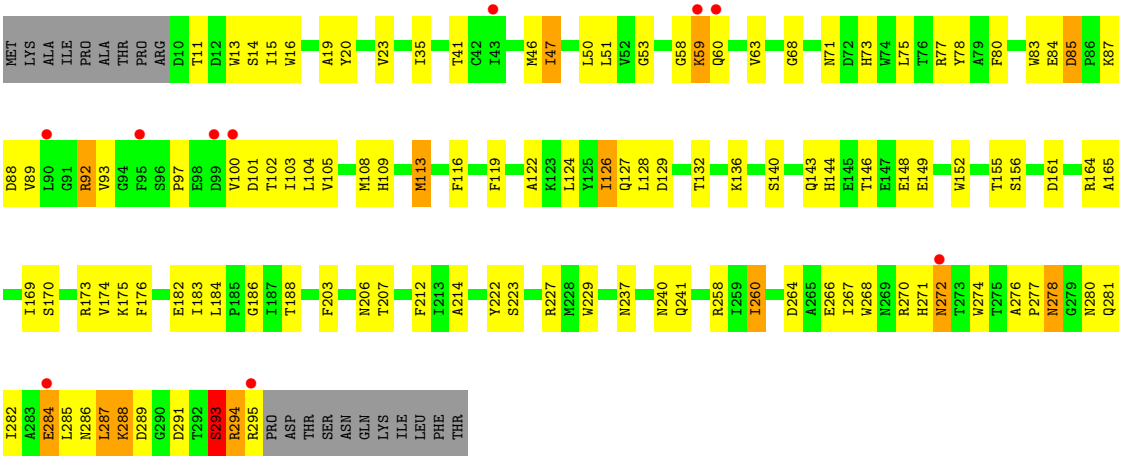
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain G:



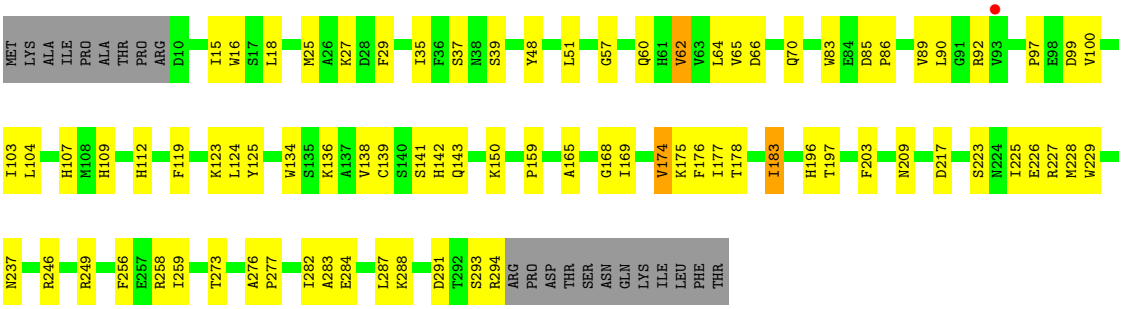
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain H:



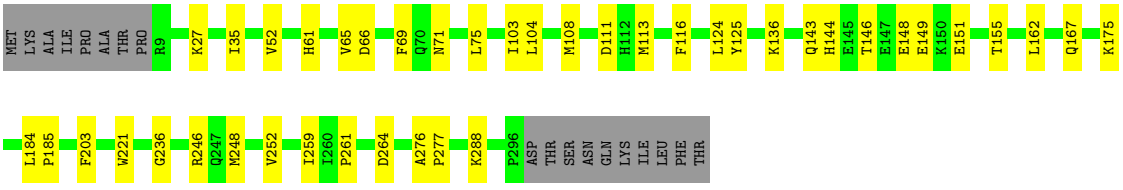
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain I:



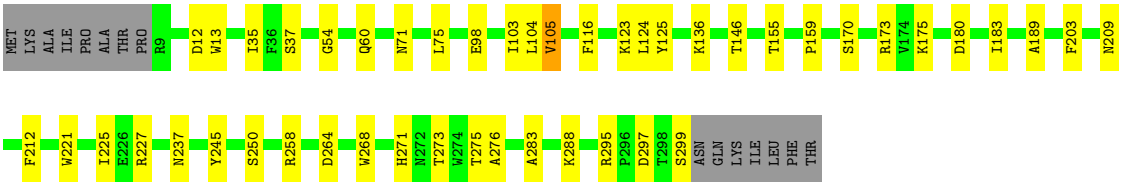
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain J:



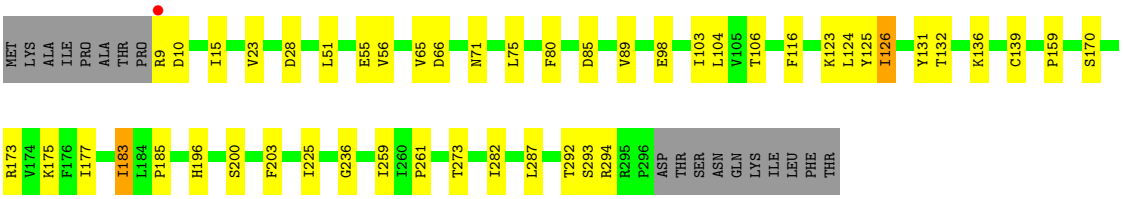
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain F:



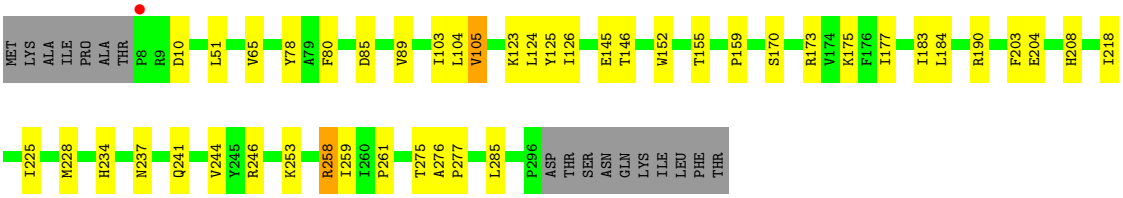
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain E:



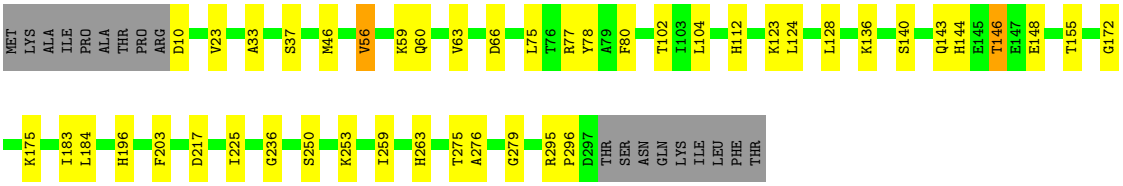
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain A:



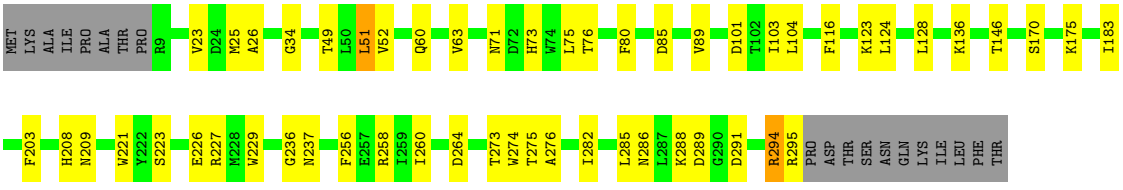
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain B:



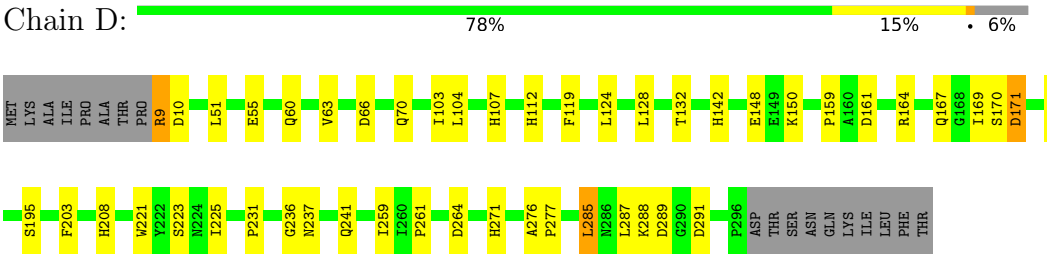
• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain C:



• Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain D:


78%
15%
6%
MET LYS ALA ILE PRO ALA THR PRO R9 D10 L51 E55 Q60 V63 D66 Q70 I103 L104 H107 H112 F119 L124 L128 T132 H142 E148 E149 K150 P159 A160 D161 R164 Q167 G168 I169 S170 D171 T178 I183 L184
S195 F203 H208 W221 Y222 S223 N224 I225 P231 G236 N237 Q241 I259 I260 P261 D264 H271 A276 P277 L285 N286 L287 K288 D289 G290 D291 P296 ASP THR SER ASN GLN LYS ILE LEU PHE THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	142.59Å 87.67Å 159.24Å 90.00° 115.79° 90.00°	Depositor
Resolution (Å)	39.96 – 2.36 39.96 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.96-2.36) 99.6 (39.96-2.36)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.168 , 0.223 0.172 , 0.225	Depositor DCC
R_{free} test set	143685 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28301	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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 30.39 % 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 1.3175e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/2396	0.67	0/3258
1	B	0.48	0/2385	0.67	0/3244
1	C	0.46	0/2380	0.64	0/3235
1	D	0.49	0/2388	0.64	0/3247
1	E	0.45	0/2388	0.63	0/3247
1	F	0.47	0/2409	0.66	0/3276
1	G	0.39	0/2388	0.60	0/3247
1	H	0.40	0/2368	0.57	0/3220
1	I	0.43	0/2358	0.62	0/3207
1	J	0.49	0/2388	0.65	0/3247
1	K	0.47	0/2377	0.66	0/3233
1	L	0.43	0/2380	0.61	0/3235
All	All	0.46	0/28605	0.63	0/38896

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

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	2324	0	2166	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2314	0	2149	42	0
1	C	2310	0	2151	41	0
1	D	2317	0	2158	36	0
1	E	2317	0	2158	37	0
1	F	2338	0	2174	27	0
1	G	2317	0	2158	40	0
1	H	2298	0	2135	101	0
1	I	2288	0	2125	80	0
1	J	2317	0	2158	37	0
1	K	2306	0	2145	94	0
1	L	2310	0	2151	60	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
2	C	6	8	8	1	0
2	D	6	8	8	0	0
2	E	6	8	8	0	0
2	F	12	16	16	0	0
2	G	6	8	8	0	0
2	H	6	8	8	0	0
2	I	6	8	7	0	0
2	J	6	8	8	0	0
2	K	6	8	7	0	0
2	L	6	8	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	56	0	0	1	0
4	B	61	0	0	0	0
4	C	37	0	0	1	0
4	D	37	0	0	1	0
4	E	33	0	0	1	0
4	F	37	0	0	1	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	8	0	0	2	0
4	I	14	0	0	0	0
4	J	34	0	0	0	0
4	K	5	0	0	0	0
4	L	13	0	0	1	0
All	All	28197	104	25930	563	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 10.

All (563) 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:E:123:LYS:HD3	1:E:175:LYS:HE2	1.31	1.12
1:I:57:GLY:HA2	1:C:295:ARG:HE	1.08	1.06
1:L:143:GLN:NE2	1:K:246:ARG:HD3	1.74	1.02
1:L:96:SER:HB2	1:L:98:GLU:OE1	1.64	0.96
1:H:100:VAL:HG23	1:H:122:ALA:HB2	1.49	0.93
1:I:48:TYR:OH	1:I:89:VAL:HG21	1.69	0.91
1:I:246:ARG:HD3	1:J:143:GLN:HE22	1.36	0.89
1:L:17:SER:HB3	1:L:47:ILE:HD11	1.55	0.88
1:H:169:ILE:HG23	1:I:139:CYS:SG	2.14	0.88
1:K:208:HIS:HB2	1:K:288:LYS:HE3	1.55	0.87
1:I:123:LYS:HD2	1:I:175:LYS:HE2	1.58	0.86
1:L:143:GLN:HE21	1:K:246:ARG:HD3	1.39	0.85
1:I:27:LYS:HD2	1:I:39:SER:HB3	1.60	0.83
1:C:73:HIS:O	1:C:76:THR:HG22	1.79	0.82
1:I:57:GLY:HA2	1:C:295:ARG:NE	1.93	0.81
1:I:143:GLN:HE22	1:J:246:ARG:HD3	1.46	0.80
1:K:288:LYS:HE2	1:K:288:LYS:HA	1.63	0.80
1:I:246:ARG:HD3	1:J:143:GLN:NE2	1.97	0.80
1:H:78:TYR:HB2	1:H:80:PHE:CE2	2.17	0.79
1:E:123:LYS:HD3	1:E:175:LYS:CE	2.12	0.79
1:K:105:VAL:HG21	1:K:124:LEU:HD21	1.65	0.79
1:I:100:VAL:HG11	1:I:119:PHE:HD2	1.48	0.78
1:J:103:ILE:HB	1:J:124:LEU:HD23	1.66	0.77
1:H:146:THR:HG23	1:H:149:GLU:HG3	1.66	0.77
1:I:143:GLN:NE2	1:J:246:ARG:HD3	1.99	0.77
1:A:123:LYS:HG2	1:A:175:LYS:HE2	1.67	0.76
1:L:146:THR:HG23	1:L:149:GLU:H	1.50	0.76
1:E:116:PHE:HE1	1:E:173:ARG:HH12	1.29	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:ASN:OD1	1:J:75:LEU:HD11	1.84	0.76
1:H:169:ILE:HD13	1:H:174:VAL:CG1	2.16	0.75
1:L:51:LEU:HB2	1:L:63:VAL:CG2	2.16	0.75
1:K:100:VAL:HG11	1:K:119:PHE:CD2	2.22	0.75
1:K:100:VAL:HG11	1:K:119:PHE:HD2	1.51	0.75
1:I:100:VAL:HG11	1:I:119:PHE:CD2	2.20	0.75
1:I:60:GLN:HG2	1:C:60:GLN:HB2	1.67	0.74
1:I:97:PRO:O	1:I:100:VAL:HG12	1.87	0.74
1:H:222:TYR:OH	1:H:267:ILE:HD13	1.86	0.74
1:C:227:ARG:NH1	1:D:148:GLU:OE2	2.20	0.74
1:H:15:ILE:HG12	1:H:51:LEU:HD22	1.69	0.74
1:H:165:ALA:O	1:H:169:ILE:HG12	1.89	0.73
1:H:11:THR:HG21	1:H:186:GLY:HA3	1.70	0.73
1:I:288:LYS:HG2	1:I:291:ASP:OD2	1.89	0.73
1:H:23:VAL:HG12	1:H:80:PHE:CD1	2.23	0.73
1:E:103:ILE:HB	1:E:124:LEU:HD23	1.69	0.72
1:I:60:GLN:O	1:I:60:GLN:HG3	1.89	0.72
1:C:103:ILE:HB	1:C:124:LEU:HD23	1.70	0.72
1:L:242:ILE:HD11	1:K:152:TRP:CE3	2.25	0.72
1:I:226:GLU:HG2	1:I:256:PHE:CD2	2.24	0.72
1:H:214:ALA:HA	1:H:260:ILE:HG13	1.71	0.71
1:H:140:SER:O	1:H:143:GLN:HG2	1.89	0.71
1:H:129:ASP:HA	1:H:132:THR:HG22	1.71	0.71
1:H:15:ILE:HG22	1:H:285:LEU:HD13	1.72	0.71
1:I:293:SER:O	1:I:294:ARG:C	2.29	0.71
1:I:226:GLU:HG2	1:I:256:PHE:CE2	2.26	0.70
1:I:57:GLY:CA	1:C:295:ARG:HE	1.96	0.70
1:I:62:VAL:CG2	1:I:100:VAL:HA	2.21	0.70
1:G:183:ILE:HD12	1:G:184:LEU:N	2.06	0.69
1:K:12:ASP:HB2	1:K:288:LYS:HG3	1.72	0.69
1:B:10:ASP:O	1:B:56:VAL:HG12	1.93	0.69
1:A:105:VAL:HG13	1:A:125:TYR:O	1.93	0.69
1:K:73:HIS:O	1:K:76:THR:HG22	1.93	0.68
1:K:23:VAL:HG22	1:K:80:PHE:CD2	2.27	0.68
1:H:169:ILE:HD13	1:H:174:VAL:HG13	1.76	0.68
1:I:35:ILE:HG21	1:I:227:ARG:HH21	1.59	0.68
1:K:248:MET:O	1:K:252:VAL:HG12	1.93	0.68
1:G:183:ILE:HD12	1:G:184:LEU:H	1.56	0.68
1:I:103:ILE:HB	1:I:124:LEU:HD12	1.75	0.67
1:K:50:LEU:CD2	1:K:52:VAL:HG23	2.25	0.67
1:B:123:LYS:HE2	1:B:172:GLY:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:HIS:CE1	1:D:112:HIS:CE1	2.83	0.67
1:K:208:HIS:HB2	1:K:288:LYS:CE	2.25	0.67
1:D:104:LEU:HD22	1:D:183:ILE:HD12	1.76	0.67
1:F:170:SER:HB2	1:A:159:PRO:HB2	1.77	0.67
1:H:51:LEU:O	1:H:63:VAL:HG22	1.95	0.66
1:E:170:SER:HB2	1:D:159:PRO:HB2	1.76	0.66
1:L:183:ILE:HD12	1:L:184:LEU:H	1.61	0.66
1:D:9:ARG:HA	1:D:9:ARG:NE	2.09	0.66
1:G:246:ARG:HD3	1:H:144:HIS:NE2	2.10	0.66
1:H:294:ARG:HH21	1:H:295:ARG:HB3	1.60	0.65
1:K:136:LYS:HB3	1:K:136:LYS:HZ2	1.60	0.65
1:H:20:TYR:CZ	1:H:68:GLY:HA2	2.31	0.65
1:E:116:PHE:HE1	1:E:173:ARG:NH1	1.95	0.65
1:E:126:ILE:HD11	1:E:131:TYR:HB2	1.79	0.65
1:K:288:LYS:HB3	1:K:288:LYS:HZ3	1.61	0.64
1:L:84:GLU:OE2	1:L:92:ARG:NH2	2.29	0.64
1:H:100:VAL:CG2	1:H:119:PHE:HB3	2.28	0.64
1:K:228:MET:HE3	1:K:249:ARG:HE	1.62	0.64
1:H:13:TRP:HB2	1:H:207:THR:HG22	1.79	0.64
1:H:116:PHE:HE1	1:H:173:ARG:HE	1.46	0.64
1:H:288:LYS:O	1:H:291:ASP:HB2	1.98	0.64
1:H:294:ARG:O	1:H:295:ARG:C	2.37	0.64
1:B:128:LEU:HD22	1:C:136:LYS:HD3	1.79	0.64
1:K:288:LYS:HE2	1:K:288:LYS:CA	2.28	0.63
1:L:35:ILE:HG23	1:L:229:TRP:CZ2	2.33	0.63
1:G:228:MET:HE1	1:G:249:ARG:HD2	1.79	0.63
1:F:103:ILE:HB	1:F:124:LEU:HD23	1.81	0.63
1:F:268:TRP:HA	1:F:273:THR:HG21	1.80	0.63
1:D:70:GLN:HG2	4:D:512:HOH:O	1.97	0.63
1:I:16:TRP:NE1	1:I:284:GLU:HG3	2.13	0.63
1:H:278:ASN:H	1:H:278:ASN:HD22	1.45	0.63
1:H:85:ASP:O	1:H:89:VAL:HG23	1.98	0.62
1:D:161:ASP:OD1	1:D:164:ARG:NH1	2.33	0.62
1:K:228:MET:CE	1:K:249:ARG:HE	2.12	0.62
1:H:23:VAL:HG12	1:H:80:PHE:CE1	2.34	0.62
1:H:276:ALA:HB1	1:H:277:PRO:CD	2.29	0.62
1:G:276:ALA:HB1	1:G:277:PRO:HD2	1.80	0.62
1:A:78:TYR:HB2	1:A:80:PHE:CE2	2.36	0.61
1:A:183:ILE:HG22	1:A:184:LEU:HD22	1.82	0.61
1:B:146:THR:HB	1:B:148:GLU:OE1	2.00	0.61
1:B:250:SER:O	1:B:253:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:PRO:HB2	1:D:170:SER:HB2	1.82	0.61
1:L:252:VAL:HG21	1:L:258:ARG:HB2	1.81	0.61
1:H:97:PRO:O	1:H:100:VAL:HG22	2.00	0.60
1:L:37:SER:OG	1:K:28:ASP:OD1	2.20	0.60
1:F:116:PHE:HE1	1:F:173:ARG:HH12	1.49	0.60
1:L:51:LEU:HB2	1:L:63:VAL:HG22	1.82	0.60
1:K:50:LEU:HD21	1:K:52:VAL:HG23	1.83	0.60
1:H:276:ALA:HB1	1:H:277:PRO:HD2	1.82	0.60
1:L:143:GLN:HE22	1:K:246:ARG:HD3	1.62	0.60
1:K:274:TRP:CH2	1:K:284:GLU:HB2	2.37	0.60
1:D:104:LEU:HB3	1:D:203:PHE:CZ	2.37	0.60
1:K:104:LEU:HB3	1:K:203:PHE:CZ	2.37	0.59
1:F:271:HIS:O	1:F:273:THR:HG23	2.02	0.59
1:H:128:LEU:HD21	1:I:136:LYS:HE2	1.84	0.59
1:B:275:THR:HG22	1:B:276:ALA:O	2.02	0.59
1:D:9:ARG:HE	1:D:10:ASP:H	1.50	0.59
1:K:208:HIS:H	1:K:288:LYS:HD3	1.66	0.59
1:L:148:GLU:OE2	1:K:227:ARG:NH1	2.36	0.59
1:I:62:VAL:HG23	1:I:100:VAL:HA	1.84	0.59
1:B:136:LYS:HE2	1:C:128:LEU:CD2	2.32	0.59
1:D:9:ARG:HD3	1:D:55:GLU:OE2	2.03	0.59
1:K:284:GLU:OE1	1:K:287:LEU:HD11	2.03	0.59
1:D:104:LEU:CD2	1:D:183:ILE:HD12	2.32	0.59
1:K:287:LEU:CD1	1:K:293:SER:HA	2.33	0.58
1:H:103:ILE:HB	1:H:124:LEU:HD23	1.85	0.58
1:H:103:ILE:HG13	1:H:122:ALA:HB1	1.85	0.58
1:K:33:ALA:O	1:K:37:SER:HB3	2.03	0.58
1:J:146:THR:HB	1:J:148:GLU:OE1	2.03	0.58
1:H:293:SER:OG	1:H:294:ARG:N	2.34	0.58
1:B:123:LYS:HD2	1:B:175:LYS:HZ2	1.67	0.58
1:B:128:LEU:CD2	1:C:136:LYS:HD3	2.33	0.58
2:C:401:GOL:H11	4:C:508:HOH:O	2.03	0.58
1:I:104:LEU:HD22	1:I:183:ILE:HD12	1.85	0.58
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.69	0.58
1:G:103:ILE:HB	1:G:124:LEU:HD12	1.86	0.57
1:F:275:THR:HG22	1:F:276:ALA:O	2.04	0.57
1:G:35:ILE:HG21	1:G:227:ARG:HH21	1.69	0.57
1:C:25:MET:HE2	1:C:26:ALA:H	1.69	0.57
1:K:50:LEU:HD21	1:K:52:VAL:CG2	2.34	0.57
1:H:169:ILE:HD13	1:H:174:VAL:HG11	1.85	0.57
1:L:92:ARG:NH1	4:L:501:HOH:O	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:GLU:CD	1:L:92:ARG:HH22	2.07	0.57
1:K:252:VAL:O	1:K:252:VAL:HG22	2.04	0.57
1:H:105:VAL:CG2	1:H:124:LEU:HD22	2.35	0.57
1:C:237:ASN:HA	1:D:236:GLY:O	2.04	0.56
1:L:252:VAL:CG2	1:L:258:ARG:HB2	2.36	0.56
1:I:104:LEU:HB3	1:I:203:PHE:CZ	2.39	0.56
1:C:275:THR:HG22	1:C:276:ALA:O	2.04	0.56
1:H:63:VAL:HG11	1:H:184:LEU:HD13	1.86	0.56
1:L:167:GLN:HG2	1:G:163:ILE:HD13	1.87	0.56
1:H:63:VAL:HG12	1:H:102:THR:HB	1.88	0.56
1:K:228:MET:CE	1:K:245:TYR:HB3	2.36	0.56
1:I:246:ARG:HE	1:J:144:HIS:HE1	1.54	0.56
1:E:139:CYS:SG	1:D:169:ILE:HG23	2.46	0.56
1:K:225:ILE:O	1:K:228:MET:HE3	2.05	0.56
1:C:34:GLY:HA3	1:C:229:TRP:HZ2	1.70	0.56
1:L:183:ILE:HD12	1:L:184:LEU:N	2.21	0.55
1:E:55:GLU:HG3	1:E:185:PRO:CB	2.36	0.55
1:D:104:LEU:HD22	1:D:183:ILE:CD1	2.36	0.55
1:L:22:GLN:O	1:L:80:PHE:HA	2.06	0.55
1:E:287:LEU:HD11	1:E:293:SER:HA	1.87	0.55
1:D:288:LYS:HG2	1:D:291:ASP:OD2	2.07	0.55
1:A:218:ILE:HG21	1:A:244:VAL:HG11	1.89	0.55
1:K:50:LEU:HD23	1:K:51:LEU:N	2.22	0.54
1:H:278:ASN:HD22	1:H:278:ASN:N	2.04	0.54
1:I:125:TYR:HD2	1:I:177:ILE:HD11	1.72	0.54
1:K:97:PRO:O	1:K:100:VAL:HG12	2.07	0.54
1:K:105:VAL:HG21	1:K:124:LEU:CD2	2.37	0.54
1:G:246:ARG:HD2	1:H:143:GLN:OE1	2.05	0.54
1:D:103:ILE:HB	1:D:124:LEU:HD12	1.89	0.54
1:E:15:ILE:HG12	1:E:51:LEU:CD2	2.38	0.54
1:K:252:VAL:HG21	1:K:258:ARG:HB2	1.88	0.54
1:K:128:LEU:HD21	1:J:136:LYS:HD2	1.90	0.54
1:K:77:ARG:O	1:K:78:TYR:HB2	2.07	0.54
1:B:136:LYS:HE2	1:C:128:LEU:HD21	1.90	0.54
1:K:287:LEU:HD11	1:K:293:SER:HA	1.89	0.54
1:H:237:ASN:HB3	1:H:240:ASN:HB2	1.90	0.54
1:C:274:TRP:CZ2	1:C:294:ARG:HG3	2.43	0.53
1:B:59:LYS:HG3	1:B:60:GLN:N	2.23	0.53
1:G:52:VAL:O	1:G:288:LYS:NZ	2.40	0.53
1:A:103:ILE:HB	1:A:124:LEU:HD12	1.89	0.53
1:L:188:THR:HG23	1:L:204:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:LEU:HB3	1:E:203:PHE:CZ	2.44	0.53
1:K:284:GLU:CD	1:K:287:LEU:HD11	2.29	0.53
1:F:116:PHE:HE1	1:F:173:ARG:NH1	2.07	0.53
1:L:103:ILE:HB	1:L:124:LEU:HD12	1.91	0.53
1:L:123:LYS:HG2	1:L:175:LYS:HE2	1.91	0.53
1:G:104:LEU:HB3	1:G:203:PHE:CZ	2.44	0.53
1:L:37:SER:OG	1:K:28:ASP:OD2	2.26	0.52
1:G:177:ILE:HD11	1:G:183:ILE:HG21	1.90	0.52
1:H:53:GLY:HA2	1:H:60:GLN:HG3	1.91	0.52
1:I:196:HIS:ND1	1:I:197:THR:HG23	2.25	0.52
1:K:12:ASP:CB	1:K:288:LYS:HG3	2.39	0.52
1:E:55:GLU:HG3	1:E:185:PRO:HB3	1.92	0.52
1:L:14:SER:OG	1:L:288:LYS:HG2	2.10	0.52
1:I:225:ILE:HD11	1:I:249:ARG:HG3	1.90	0.52
1:H:23:VAL:CG1	1:H:80:PHE:CE1	2.93	0.52
1:H:264:ASP:O	1:H:267:ILE:HG22	2.10	0.52
1:H:287:LEU:HD22	1:H:293:SER:HA	1.92	0.51
1:G:146:THR:HG23	1:G:149:GLU:OE2	2.10	0.51
1:I:176:PHE:O	1:I:177:ILE:HD13	2.11	0.51
1:D:195:SER:O	1:D:236:GLY:HA3	2.10	0.51
1:G:132:THR:O	1:G:136:LYS:HD3	2.10	0.51
1:H:129:ASP:HA	1:H:132:THR:CG2	2.40	0.51
1:C:209:ASN:ND2	1:C:286:ASN:OD1	2.37	0.51
1:D:225:ILE:HD13	1:D:259:ILE:HD13	1.92	0.51
1:H:19:ALA:O	1:H:280:ASN:HB3	2.10	0.51
1:I:134:TRP:O	1:I:138:VAL:HG23	2.10	0.51
1:G:68:GLY:O	1:G:114:GLY:O	2.29	0.51
1:K:78:TYR:HB2	1:K:80:PHE:CE1	2.46	0.51
1:K:85:ASP:O	1:K:89:VAL:HG23	2.10	0.51
1:K:272:ASN:CG	1:K:274:TRP:HZ3	2.14	0.51
1:I:249:ARG:HG2	1:I:256:PHE:HE1	1.75	0.51
1:J:144:HIS:CD2	1:J:149:GLU:HB3	2.46	0.51
1:B:104:LEU:HB3	1:B:203:PHE:CZ	2.46	0.51
1:K:252:VAL:CG2	1:K:258:ARG:HB2	2.40	0.51
1:H:284:GLU:OE1	1:H:287:LEU:HD21	2.11	0.51
1:I:273:THR:HG23	1:I:282:ILE:O	2.11	0.51
1:L:170:SER:HB2	1:G:159:PRO:HB2	1.93	0.50
1:E:104:LEU:HD22	1:E:183:ILE:HD12	1.93	0.50
1:J:104:LEU:HB3	1:J:203:PHE:CZ	2.47	0.50
1:C:226:GLU:HG2	1:C:256:PHE:CD2	2.46	0.50
1:L:9:ARG:HB3	1:L:9:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:VAL:CG1	1:I:119:PHE:HD2	2.23	0.50
1:K:274:TRP:CH2	1:K:295:ARG:HB2	2.47	0.50
1:H:14:SER:HA	1:H:286:ASN:O	2.11	0.50
1:I:225:ILE:HD13	1:I:259:ILE:HD13	1.93	0.50
1:E:55:GLU:CG	1:E:185:PRO:HB3	2.42	0.50
1:E:85:ASP:O	1:E:89:VAL:HG23	2.11	0.50
1:A:228:MET:HE1	1:B:144:HIS:HE1	1.77	0.50
1:K:108:MET:SD	1:K:126:ILE:CD1	3.00	0.50
1:C:49:THR:HG22	1:C:51:LEU:CD1	2.42	0.50
1:H:274:TRP:HZ2	1:H:294:ARG:HD3	1.77	0.49
1:B:140:SER:O	1:B:143:GLN:HG2	2.12	0.49
1:B:23:VAL:HG12	1:B:46:MET:HE3	1.94	0.49
1:D:142:HIS:HA	1:D:150:LYS:HE2	1.93	0.49
1:H:75:LEU:HD21	1:H:83:TRP:HB2	1.93	0.49
1:F:209:ASN:O	1:F:258:ARG:NH2	2.45	0.49
1:A:85:ASP:O	1:A:89:VAL:HG23	2.13	0.49
1:J:27:LYS:HG2	1:J:221:TRP:HH2	1.77	0.49
1:J:248:MET:O	1:J:252:VAL:HG22	2.12	0.49
1:E:125:TYR:HB3	1:E:177:ILE:HD11	1.94	0.49
1:H:146:THR:CG2	1:H:149:GLU:HG3	2.39	0.49
1:H:274:TRP:HE1	1:H:294:ARG:CZ	2.25	0.49
1:G:177:ILE:CD1	1:G:183:ILE:HG21	2.43	0.49
1:I:109:HIS:ND1	1:I:196:HIS:HE1	2.10	0.49
1:E:10:ASP:O	1:E:56:VAL:HG23	2.13	0.49
1:B:63:VAL:HG21	1:B:184:LEU:CD1	2.43	0.49
1:L:268:TRP:CE2	1:L:281:GLN:HB2	2.47	0.49
1:I:86:PRO:HA	1:I:89:VAL:HG22	1.93	0.49
1:H:73:HIS:HE1	4:H:506:HOH:O	1.96	0.48
1:F:159:PRO:HB2	1:A:170:SER:HB3	1.95	0.48
1:C:226:GLU:HG2	1:C:256:PHE:CE2	2.48	0.48
1:I:16:TRP:CD1	1:I:284:GLU:HG3	2.48	0.48
1:F:71:ASN:OD1	1:F:75:LEU:HD12	2.13	0.48
1:A:177:ILE:HD11	1:A:183:ILE:HG13	1.96	0.48
1:L:43:ILE:O	1:L:43:ILE:HG13	2.12	0.48
1:C:25:MET:HA	1:C:25:MET:CE	2.43	0.48
1:G:284:GLU:OE2	1:G:287:LEU:HD11	2.13	0.48
1:J:116:PHE:CG	1:J:124:LEU:HD11	2.48	0.48
1:A:275:THR:HG22	1:A:276:ALA:O	2.14	0.48
1:L:98:GLU:H	1:L:98:GLU:CD	2.16	0.48
1:F:221:TRP:HA	1:F:264:ASP:HB2	1.96	0.48
1:I:25:MET:HE1	1:I:29:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:TRP:CD1	1:H:284:GLU:HB2	2.49	0.48
1:L:63:VAL:HG11	1:L:184:LEU:HD13	1.96	0.48
1:K:128:LEU:CD2	1:J:136:LYS:HD2	2.44	0.48
1:K:274:TRP:CE3	1:K:295:ARG:HG3	2.49	0.48
1:A:258:ARG:HG2	1:A:258:ARG:NH1	2.28	0.48
1:H:100:VAL:HG21	1:H:119:PHE:HB3	1.95	0.47
1:H:271:HIS:NE2	1:H:285:LEU:HD23	2.29	0.47
1:J:125:TYR:CZ	1:J:175:LYS:HD2	2.49	0.47
1:C:25:MET:HA	1:C:25:MET:HE3	1.95	0.47
1:I:16:TRP:HA	1:I:283:ALA:O	2.14	0.47
1:A:225:ILE:HD13	1:A:259:ILE:HD13	1.96	0.47
1:A:228:MET:CE	1:B:144:HIS:CE1	2.97	0.47
1:K:12:ASP:OD1	1:K:56:VAL:HG22	2.14	0.47
1:C:291:ASP:OD2	1:C:295:ARG:HD2	2.13	0.47
1:L:252:VAL:HG21	1:L:258:ARG:CB	2.44	0.47
1:H:146:THR:OG1	1:H:148:GLU:HG2	2.14	0.47
1:A:190:ARG:NE	1:A:204:GLU:OE2	2.43	0.47
1:K:65:VAL:O	1:K:66:ASP:HB2	2.14	0.47
1:K:108:MET:HG3	1:K:126:ILE:HD12	1.96	0.47
1:K:228:MET:HE1	1:K:245:TYR:HB3	1.96	0.47
1:H:59:LYS:HA	1:H:59:LYS:HD3	1.48	0.47
1:H:108:MET:SD	1:H:126:ILE:CD1	3.02	0.47
1:L:182:GLU:HA	1:L:188:THR:HA	1.96	0.47
1:H:241:GLN:NE2	4:H:501:HOH:O	2.46	0.47
1:I:223:SER:O	1:I:227:ARG:HB2	2.14	0.47
1:B:46:MET:HE2	1:B:263:HIS:HD1	1.79	0.47
1:B:123:LYS:HD2	1:B:175:LYS:HE3	1.96	0.47
1:K:100:VAL:CG1	1:K:119:PHE:HD2	2.24	0.47
1:K:109:HIS:CD2	1:K:156:SER:HB3	2.50	0.47
1:L:63:VAL:HG11	1:L:184:LEU:CD1	2.45	0.47
1:K:209:ASN:O	1:K:258:ARG:NH2	2.39	0.47
1:I:104:LEU:CD2	1:I:183:ILE:HD12	2.44	0.47
1:F:273:THR:HG22	1:F:283:ALA:HA	1.97	0.47
1:C:85:ASP:O	1:C:89:VAL:HG23	2.15	0.47
1:L:168:GLY:HA2	1:L:173:ARG:HG2	1.96	0.46
1:L:252:VAL:CG2	1:L:258:ARG:CB	2.93	0.46
1:K:47:ILE:HD11	1:K:268:TRP:CH2	2.50	0.46
1:H:223:SER:O	1:H:227:ARG:HB2	2.15	0.46
1:H:272:ASN:ND2	1:H:272:ASN:H	2.14	0.46
1:K:273:THR:HG22	1:K:274:TRP:O	2.15	0.46
1:G:15:ILE:HG12	1:G:51:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ILE:HG13	1:F:245:TYR:HB3	1.97	0.46
1:E:106:THR:O	1:E:200:SER:HA	2.15	0.46
1:H:161:ASP:OD1	1:H:164:ARG:NH2	2.49	0.46
1:I:165:ALA:O	1:I:169:ILE:HG12	2.15	0.46
1:F:104:LEU:HB3	1:F:203:PHE:CZ	2.50	0.46
1:E:71:ASN:OD1	1:E:75:LEU:HD12	2.15	0.46
1:L:23:VAL:HG23	1:L:80:PHE:CD1	2.50	0.46
1:L:146:THR:CG2	1:L:149:GLU:HG3	2.46	0.46
1:L:276:ALA:HB1	1:L:277:PRO:HD2	1.97	0.46
1:K:228:MET:HE3	1:K:249:ARG:NE	2.28	0.46
1:H:19:ALA:HA	1:H:47:ILE:HG22	1.98	0.46
1:H:152:TRP:HA	1:H:155:THR:HG23	1.97	0.46
1:F:175:LYS:NZ	4:F:502:HOH:O	2.46	0.46
1:L:37:SER:OG	1:K:28:ASP:CG	2.53	0.46
1:F:13:TRP:CZ2	1:F:54:GLY:HA2	2.51	0.46
1:C:260:ILE:HG12	1:C:285:LEU:HD21	1.98	0.46
1:F:98:GLU:OE1	1:F:98:GLU:N	2.48	0.46
1:A:173:ARG:HG2	4:A:550:HOH:O	2.14	0.46
1:B:225:ILE:HD13	1:B:259:ILE:HD13	1.97	0.46
1:C:52:VAL:CG1	1:C:295:ARG:HH12	2.29	0.46
1:K:12:ASP:HB2	1:K:288:LYS:CG	2.43	0.46
1:H:35:ILE:HG23	1:H:229:TRP:CH2	2.51	0.46
1:H:16:TRP:CZ2	1:H:287:LEU:HD23	2.51	0.46
1:E:292:THR:O	1:E:294:ARG:NH1	2.49	0.46
1:G:195:SER:O	1:G:236:GLY:HA3	2.16	0.46
1:H:11:THR:HG22	1:H:206:ASN:O	2.15	0.46
1:H:100:VAL:CG2	1:H:122:ALA:HB2	2.33	0.46
1:H:169:ILE:CD1	1:H:174:VAL:HG11	2.46	0.46
1:H:183:ILE:HD12	1:H:183:ILE:HA	1.77	0.46
1:J:27:LYS:CG	1:J:221:TRP:HH2	2.29	0.46
1:J:65:VAL:O	1:J:66:ASP:HB2	2.16	0.46
1:L:65:VAL:O	1:L:66:ASP:HB2	2.15	0.46
1:K:93:VAL:O	1:K:294:ARG:NH1	2.48	0.46
1:K:163:ILE:HD13	1:J:167:GLN:HG2	1.98	0.46
1:K:286:ASN:ND2	1:K:288:LYS:HG2	2.31	0.46
1:H:58:GLY:O	1:H:59:LYS:C	2.54	0.46
1:B:66:ASP:OD2	1:B:112:HIS:ND1	2.32	0.46
1:L:143:GLN:HE21	1:K:246:ARG:CD	2.21	0.45
1:I:176:PHE:C	1:I:177:ILE:HD13	2.36	0.45
1:E:183:ILE:H	1:E:183:ILE:HG12	1.56	0.45
1:K:228:MET:CE	1:K:249:ARG:NE	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LEU:HB3	1:H:203:PHE:CZ	2.51	0.45
1:J:52:VAL:HA	1:J:61:HIS:O	2.16	0.45
1:L:242:ILE:HD11	1:K:152:TRP:CZ3	2.52	0.45
1:E:170:SER:HB2	1:D:159:PRO:CB	2.43	0.45
1:K:136:LYS:HB3	1:K:136:LYS:NZ	2.28	0.45
1:G:44:ASN:HB3	1:G:263:HIS:O	2.16	0.45
1:J:136:LYS:HB3	1:J:136:LYS:HE2	1.63	0.45
1:C:52:VAL:HG11	1:C:295:ARG:NH1	2.31	0.45
1:K:35:ILE:HG23	1:K:229:TRP:CZ2	2.52	0.45
1:K:183:ILE:HD11	1:K:189:ALA:HB2	1.98	0.45
1:I:27:LYS:NZ	1:I:39:SER:O	2.28	0.45
1:H:126:ILE:HG13	1:H:127:GLN:N	2.32	0.45
1:I:109:HIS:CE1	1:I:196:HIS:CE1	3.04	0.45
1:K:152:TRP:HA	1:K:155:THR:HG23	1.99	0.45
1:E:259:ILE:O	1:E:261:PRO:HD3	2.16	0.45
1:C:208:HIS:ND1	1:C:289:ASP:OD2	2.36	0.45
1:L:168:GLY:HA3	1:L:174:VAL:HG23	1.99	0.45
1:L:268:TRP:HB3	1:L:273:THR:HG21	1.99	0.45
1:G:71:ASN:OD1	1:G:75:LEU:HD12	2.17	0.45
1:H:87:LYS:HG2	1:H:97:PRO:HD2	1.99	0.45
1:A:10:ASP:OD1	1:A:208:HIS:NE2	2.50	0.45
1:K:12:ASP:OD1	1:K:208:HIS:CE1	2.69	0.45
1:I:62:VAL:HG22	1:I:99:ASP:O	2.17	0.45
1:I:143:GLN:NE2	1:J:246:ARG:CD	2.74	0.45
1:B:10:ASP:OD2	1:B:56:VAL:HG11	2.17	0.45
1:C:104:LEU:HB3	1:C:203:PHE:CZ	2.52	0.45
1:K:28:ASP:HB3	1:K:37:SER:HA	1.99	0.45
1:K:35:ILE:HG13	1:K:36:PHE:CD2	2.52	0.45
1:H:182:GLU:HA	1:H:188:THR:HA	1.97	0.45
1:I:123:LYS:HD2	1:I:175:LYS:CE	2.38	0.45
1:J:69:PHE:HB3	1:J:111:ASP:HA	2.00	0.45
1:C:209:ASN:O	1:C:258:ARG:NH2	2.50	0.45
1:I:25:MET:CE	1:I:29:PHE:CD1	3.00	0.44
1:I:104:LEU:HD22	1:I:183:ILE:CD1	2.47	0.44
1:I:237:ASN:HA	1:J:236:GLY:O	2.17	0.44
1:F:273:THR:HG22	1:F:283:ALA:CB	2.48	0.44
1:C:123:LYS:HD2	1:C:175:LYS:HE2	1.99	0.44
1:K:101:ASP:O	1:K:102:THR:HG23	2.18	0.44
1:A:152:TRP:HA	1:A:155:THR:HG23	2.00	0.44
1:D:231:PRO:HD2	1:D:241:GLN:HE22	1.82	0.44
1:H:288:LYS:O	1:H:289:ASP:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:CG1	1:A:126:ILE:HG12	2.47	0.44
1:C:291:ASP:OD1	1:C:295:ARG:HD2	2.17	0.44
1:L:132:THR:HG22	1:G:132:THR:HG22	1.98	0.44
1:J:108:MET:HG2	1:J:113:MET:SD	2.57	0.44
1:J:276:ALA:HB1	1:J:277:PRO:HD2	2.00	0.44
1:E:15:ILE:HG12	1:E:51:LEU:HD23	1.98	0.44
1:D:66:ASP:CG	1:D:112:HIS:HB3	2.37	0.44
1:K:271:HIS:O	1:K:272:ASN:C	2.55	0.44
1:F:295:ARG:NH1	1:F:299:SER:OG	2.49	0.44
1:B:295:ARG:HG2	1:B:296:PRO:O	2.18	0.44
1:L:35:ILE:HG23	1:L:229:TRP:CH2	2.52	0.44
1:L:242:ILE:CD1	1:K:152:TRP:CZ3	3.00	0.44
1:K:225:ILE:O	1:K:228:MET:CE	2.65	0.44
1:G:107:HIS:CE1	1:G:112:HIS:CD2	3.06	0.44
1:H:267:ILE:O	1:H:267:ILE:HD12	2.18	0.44
1:I:35:ILE:HG21	1:I:227:ARG:NH2	2.29	0.44
1:E:136:LYS:HD2	1:D:128:LEU:HD21	1.99	0.44
1:A:259:ILE:O	1:A:261:PRO:HD3	2.17	0.44
1:D:221:TRP:HA	1:D:264:ASP:HB2	1.99	0.44
1:H:71:ASN:HB2	1:H:83:TRP:CE3	2.52	0.44
1:H:88:ASP:O	1:H:92:ARG:HD3	2.18	0.44
1:I:18:LEU:CD1	1:I:90:LEU:HD23	2.48	0.44
1:A:104:LEU:HB3	1:A:203:PHE:CZ	2.53	0.44
1:A:228:MET:HE1	1:B:144:HIS:CE1	2.52	0.44
1:C:23:VAL:HG23	1:C:80:PHE:CD1	2.53	0.44
1:C:34:GLY:HA3	1:C:229:TRP:CZ2	2.52	0.44
1:C:71:ASN:OD1	1:C:75:LEU:HD12	2.17	0.44
1:K:291:ASP:O	1:K:292:THR:C	2.56	0.44
1:B:46:MET:HE2	1:B:263:HIS:ND1	2.33	0.44
1:D:119:PHE:CD1	1:D:119:PHE:N	2.86	0.44
1:A:123:LYS:CG	1:A:175:LYS:HE2	2.42	0.44
1:C:52:VAL:HG11	1:C:295:ARG:HH12	1.83	0.44
1:D:167:GLN:O	1:D:171:ASP:OD1	2.35	0.44
1:L:140:SER:O	1:L:143:GLN:HG2	2.18	0.43
1:K:46:MET:CE	1:K:80:PHE:HE2	2.31	0.43
1:H:16:TRP:HE3	1:H:50:LEU:HD23	1.82	0.43
1:A:237:ASN:HA	1:B:236:GLY:O	2.17	0.43
1:B:23:VAL:CG1	1:B:46:MET:HE3	2.48	0.43
1:H:16:TRP:NE1	1:H:284:GLU:HB2	2.33	0.43
1:L:85:ASP:OD1	1:L:86:PRO:HD2	2.18	0.43
1:I:107:HIS:CE1	1:I:217:ASP:OD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:GLY:C	1:I:174:VAL:HG12	2.38	0.43
1:I:169:ILE:HA	1:I:174:VAL:HG13	1.99	0.43
1:I:276:ALA:HB1	1:I:277:PRO:HD2	2.00	0.43
1:K:12:ASP:HA	1:K:207:THR:HA	2.00	0.43
1:F:212:PHE:CE2	1:F:258:ARG:HD3	2.53	0.43
1:L:37:SER:HG	1:K:28:ASP:CG	2.20	0.43
1:H:109:HIS:CG	1:H:156:SER:HB3	2.54	0.43
1:H:113:MET:HG2	1:H:113:MET:O	2.18	0.43
1:B:183:ILE:H	1:B:183:ILE:HG12	1.57	0.43
1:C:273:THR:HA	1:C:282:ILE:O	2.18	0.43
1:K:84:GLU:CD	1:K:92:ARG:HH22	2.22	0.43
1:E:125:TYR:CZ	1:E:175:LYS:HD2	2.54	0.43
1:C:221:TRP:HA	1:C:264:ASP:HB2	2.01	0.43
1:L:221:TRP:HA	1:L:264:ASP:HB2	2.01	0.43
1:I:15:ILE:HG12	1:I:51:LEU:CD2	2.49	0.43
1:J:221:TRP:HA	1:J:264:ASP:HB2	1.99	0.43
1:B:10:ASP:CG	1:B:56:VAL:HG11	2.39	0.43
1:B:78:TYR:HB2	1:B:80:PHE:CE2	2.52	0.43
1:D:271:HIS:CE1	1:D:285:LEU:HD13	2.53	0.43
1:L:242:ILE:CD1	1:K:152:TRP:CE3	3.00	0.43
1:L:294:ARG:HG3	1:L:294:ARG:HH11	1.84	0.43
1:K:126:ILE:HG13	1:K:127:GLN:N	2.34	0.43
1:K:287:LEU:HD13	1:K:293:SER:HA	2.00	0.43
1:I:119:PHE:N	1:I:119:PHE:CD1	2.87	0.43
1:K:119:PHE:CD1	1:K:119:PHE:N	2.87	0.43
1:I:92:ARG:CZ	1:I:276:ALA:HB2	2.48	0.43
1:D:276:ALA:HB1	1:D:277:PRO:HD2	2.01	0.43
1:G:23:VAL:HG23	1:G:80:PHE:CD1	2.54	0.42
1:H:63:VAL:HA	1:H:102:THR:O	2.19	0.42
1:I:57:GLY:CA	1:C:295:ARG:HG3	2.49	0.42
1:I:83:TRP:CH2	1:I:85:ASP:HA	2.54	0.42
1:D:63:VAL:HG21	1:D:184:LEU:HD13	2.00	0.42
1:H:170:SER:OG	1:I:159:PRO:HB2	2.19	0.42
1:I:65:VAL:O	1:I:66:ASP:HB2	2.19	0.42
1:J:144:HIS:HB3	1:J:149:GLU:OE1	2.19	0.42
1:L:268:TRP:CZ2	1:L:281:GLN:HB2	2.55	0.42
1:I:246:ARG:HE	1:J:144:HIS:CE1	2.33	0.42
1:E:65:VAL:O	1:E:66:ASP:HB2	2.20	0.42
1:D:51:LEU:HB2	1:D:63:VAL:HB	2.01	0.42
1:H:274:TRP:HE1	1:H:294:ARG:NE	2.18	0.42
1:I:64:LEU:O	1:I:103:ILE:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:116:PHE:HB2	1:J:124:LEU:HD21	2.00	0.42
1:E:23:VAL:HG23	1:E:80:PHE:CD1	2.54	0.42
1:G:168:GLY:HA2	1:G:173:ARG:HG2	2.00	0.42
1:H:19:ALA:HB2	1:H:268:TRP:CZ2	2.54	0.42
1:H:116:PHE:CG	1:H:124:LEU:HD11	2.55	0.42
1:F:12:ASP:CG	1:F:288:LYS:HB2	2.40	0.42
1:H:295:ARG:HE	1:H:295:ARG:HB2	1.68	0.42
1:I:246:ARG:CD	1:J:143:GLN:NE2	2.74	0.42
1:J:151:GLU:O	1:J:155:THR:HG23	2.20	0.42
1:B:33:ALA:O	1:B:37:SER:OG	2.31	0.42
1:G:228:MET:HE3	1:G:246:ARG:HG2	2.00	0.42
1:F:35:ILE:HG21	1:F:227:ARG:NH2	2.34	0.42
1:F:180:ASP:HA	1:F:189:ALA:O	2.20	0.42
1:D:9:ARG:NE	1:D:10:ASP:H	2.15	0.42
1:I:246:ARG:NE	1:J:144:HIS:HE1	2.17	0.42
1:J:259:ILE:O	1:J:261:PRO:HD3	2.20	0.42
1:B:59:LYS:C	1:B:60:GLN:HE21	2.23	0.42
1:H:23:VAL:HG13	1:H:46:MET:SD	2.60	0.42
1:F:237:ASN:HA	1:E:236:GLY:O	2.20	0.42
1:B:275:THR:HG23	1:B:279:GLY:C	2.40	0.42
1:E:132:THR:HG22	1:D:132:THR:HG22	2.01	0.42
1:G:161:ASP:OD1	1:G:164:ARG:NH1	2.53	0.41
1:H:84:GLU:CD	1:H:92:ARG:HH12	2.23	0.41
1:B:123:LYS:HD2	1:B:175:LYS:NZ	2.34	0.41
1:H:71:ASN:HB2	1:H:83:TRP:CD2	2.55	0.41
1:H:129:ASP:CA	1:H:132:THR:HG22	2.45	0.41
1:I:142:HIS:HA	1:I:150:LYS:HE2	2.01	0.41
1:B:275:THR:CG2	1:B:279:GLY:HA2	2.50	0.41
1:A:51:LEU:CD1	1:A:65:VAL:HG23	2.50	0.41
1:B:63:VAL:HG22	1:B:102:THR:HB	2.01	0.41
1:B:104:LEU:HD22	1:B:183:ILE:HD12	2.02	0.41
1:L:47:ILE:HG22	1:L:262:GLY:O	2.19	0.41
1:I:107:HIS:CE1	1:I:112:HIS:CD2	3.08	0.41
1:J:184:LEU:HB3	1:J:185:PRO:HD2	2.02	0.41
1:A:246:ARG:HE	1:B:144:HIS:CE1	2.39	0.41
1:K:23:VAL:CG2	1:K:46:MET:SD	3.08	0.41
1:H:212:PHE:CE1	1:H:258:ARG:HD2	2.55	0.41
1:I:209:ASN:O	1:I:258:ARG:NH2	2.54	0.41
1:L:125:TYR:CZ	1:L:175:LYS:HD2	2.56	0.41
1:G:18:LEU:CD2	1:G:282:ILE:HG23	2.50	0.41
1:B:196:HIS:CD2	1:B:217:ASP:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:LYS:HD2	1:G:123:LYS:N	2.36	0.41
1:G:151:GLU:O	1:G:155:THR:HG23	2.20	0.41
1:H:175:LYS:HG3	1:H:176:PHE:N	2.35	0.41
1:H:281:GLN:OE1	1:H:281:GLN:N	2.45	0.41
1:I:64:LEU:HB2	1:I:103:ILE:HG12	2.03	0.41
1:I:177:ILE:HD13	1:I:177:ILE:N	2.36	0.41
1:E:98:GLU:OE1	1:E:98:GLU:N	2.43	0.41
1:C:236:GLY:O	1:D:237:ASN:HA	2.20	0.41
1:L:276:ALA:HB1	1:L:277:PRO:CD	2.50	0.41
1:G:64:LEU:HD23	1:G:64:LEU:HA	1.82	0.41
1:G:228:MET:CE	1:H:144:HIS:CE1	3.04	0.41
1:I:35:ILE:HG23	1:I:229:TRP:CH2	2.55	0.41
1:B:148:GLU:OE1	1:B:148:GLU:N	2.35	0.41
1:C:116:PHE:CD2	1:C:124:LEU:HD11	2.55	0.41
1:K:286:ASN:HD21	1:K:288:LYS:HD2	1.86	0.41
1:F:37:SER:OG	1:E:28:ASP:OD2	2.39	0.41
1:G:168:GLY:HA3	1:G:174:VAL:HG23	2.03	0.40
1:J:162:LEU:HD23	1:J:162:LEU:HA	1.92	0.40
1:F:75:LEU:HD23	1:F:75:LEU:HA	1.87	0.40
1:A:125:TYR:CZ	1:A:175:LYS:HD2	2.56	0.40
1:A:234:HIS:CG	1:A:241:GLN:HE22	2.39	0.40
1:D:259:ILE:O	1:D:261:PRO:HD3	2.21	0.40
1:K:50:LEU:CD2	1:K:50:LEU:C	2.90	0.40
1:G:231:PRO:HD2	1:G:241:GLN:HE22	1.86	0.40
1:E:196:HIS:HE1	4:E:510:HOH:O	2.03	0.40
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.82	0.40
1:D:208:HIS:ND1	1:D:289:ASP:OD2	2.54	0.40
1:K:127:GLN:HA	1:K:177:ILE:O	2.21	0.40
1:G:15:ILE:HG12	1:G:51:LEU:CD2	2.51	0.40
1:G:228:MET:HE3	1:H:144:HIS:CE1	2.56	0.40
1:G:228:MET:CE	1:G:249:ARG:HD2	2.47	0.40
1:H:294:ARG:HE	1:H:295:ARG:HB3	1.86	0.40
1:I:225:ILE:O	1:I:249:ARG:NH1	2.52	0.40
1:E:225:ILE:HD13	1:E:259:ILE:HD13	2.03	0.40
1:L:146:THR:HG22	1:L:149:GLU:CD	2.42	0.40
1:K:91:GLY:HA2	1:K:95:PHE:O	2.21	0.40
1:G:66:ASP:OD2	1:G:112:HIS:ND1	2.50	0.40
1:I:228:MET:HG3	1:J:144:HIS:CD2	2.56	0.40
1:A:276:ALA:HB1	1:A:277:PRO:HD2	2.02	0.40
1:G:74:TRP:CZ2	1:G:158:ASP:HB2	2.56	0.40
1:F:105:VAL:HG13	1:F:125:TYR:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:THR:HA	1:E:282:ILE:O	2.22	0.40
1:B:59:LYS:HE2	1:B:59:LYS:HB2	1.92	0.40

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	287/306 (94%)	278 (97%)	9 (3%)	0	100	100
1	B	286/306 (94%)	273 (96%)	13 (4%)	0	100	100
1	C	285/306 (93%)	272 (95%)	13 (5%)	0	100	100
1	D	286/306 (94%)	275 (96%)	11 (4%)	0	100	100
1	E	286/306 (94%)	276 (96%)	10 (4%)	0	100	100
1	F	289/306 (94%)	278 (96%)	11 (4%)	0	100	100
1	G	286/306 (94%)	274 (96%)	12 (4%)	0	100	100
1	H	284/306 (93%)	261 (92%)	22 (8%)	1 (0%)	30	34
1	I	283/306 (92%)	271 (96%)	12 (4%)	0	100	100
1	J	286/306 (94%)	277 (97%)	9 (3%)	0	100	100
1	K	285/306 (93%)	264 (93%)	20 (7%)	1 (0%)	30	34
1	L	285/306 (93%)	274 (96%)	11 (4%)	0	100	100
All	All	3428/3672 (93%)	3273 (96%)	153 (4%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	289	ASP
1	H	293	SER

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	246/261 (94%)	240 (98%)	6 (2%)	44 55
1	B	245/261 (94%)	240 (98%)	5 (2%)	50 63
1	C	244/261 (94%)	235 (96%)	9 (4%)	29 38
1	D	245/261 (94%)	238 (97%)	7 (3%)	37 48
1	E	245/261 (94%)	242 (99%)	3 (1%)	67 80
1	F	248/261 (95%)	239 (96%)	9 (4%)	30 39
1	G	245/261 (94%)	230 (94%)	15 (6%)	15 17
1	H	242/261 (93%)	220 (91%)	22 (9%)	7 7
1	I	242/261 (93%)	234 (97%)	8 (3%)	33 42
1	J	245/261 (94%)	243 (99%)	2 (1%)	79 88
1	K	244/261 (94%)	228 (93%)	16 (7%)	14 15
1	L	244/261 (94%)	236 (97%)	8 (3%)	33 42
All	All	2935/3132 (94%)	2825 (96%)	110 (4%)	29 38

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	ARG
1	L	37	SER
1	L	76	THR
1	L	82	SER
1	L	96	SER
1	L	153	VAL
1	L	188	THR
1	L	252	VAL
1	K	11	THR
1	K	12	ASP
1	K	47	ILE
1	K	50	LEU
1	K	93	VAL
1	K	102	THR

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Mol	Chain	Res	Type
1	K	124	LEU
1	K	126	ILE
1	K	146	THR
1	K	156	SER
1	K	183	ILE
1	K	253	LYS
1	K	258	ARG
1	K	274	TRP
1	K	288	LYS
1	K	292	THR
1	G	23	VAL
1	G	37	SER
1	G	43	ILE
1	G	47	ILE
1	G	56	VAL
1	G	60	GLN
1	G	76	THR
1	G	77	ARG
1	G	81	SER
1	G	98	GLU
1	G	146	THR
1	G	178	THR
1	G	288	LYS
1	G	292	THR
1	G	295	ARG
1	H	41	THR
1	H	47	ILE
1	H	59	LYS
1	H	77	ARG
1	H	85	ASP
1	H	92	ARG
1	H	93	VAL
1	H	101	ASP
1	H	113	MET
1	H	126	ILE
1	H	136	LYS
1	H	260	ILE
1	H	266	GLU
1	H	270	ARG
1	H	272	ASN
1	H	278	ASN
1	H	282	ILE

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Mol	Chain	Res	Type
1	H	284	GLU
1	H	287	LEU
1	H	288	LYS
1	H	293	SER
1	H	294	ARG
1	I	37	SER
1	I	62	VAL
1	I	70	GLN
1	I	141	SER
1	I	174	VAL
1	I	178	THR
1	I	183	ILE
1	I	287	LEU
1	J	35	ILE
1	J	288	LYS
1	F	60	GLN
1	F	105	VAL
1	F	123	LYS
1	F	136	LYS
1	F	146	THR
1	F	155	THR
1	F	183	ILE
1	F	250	SER
1	F	297	ASP
1	E	9	ARG
1	E	126	ILE
1	E	183	ILE
1	A	105	VAL
1	A	145	GLU
1	A	146	THR
1	A	253	LYS
1	A	258	ARG
1	A	285	LEU
1	B	56	VAL
1	B	77	ARG
1	B	124	LEU
1	B	146	THR
1	B	155	THR
1	C	51	LEU
1	C	63	VAL
1	C	101	ASP
1	C	146	THR

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Mol	Chain	Res	Type
1	C	170	SER
1	C	183	ILE
1	C	223	SER
1	C	288	LYS
1	C	294	ARG
1	D	9	ARG
1	D	60	GLN
1	D	171	ASP
1	D	178	THR
1	D	223	SER
1	D	285	LEU
1	D	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	143	GLN
1	G	143	GLN
1	H	71	ASN
1	H	278	ASN
1	I	143	GLN
1	I	196	HIS
1	J	143	GLN
1	D	112	HIS

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 37 ligands modelled in this entry, 24 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
2	GOL	C	401	-	5,5,5	0.51	0	5,5,5	1.29	0
2	GOL	F	402	-	5,5,5	0.87	0	5,5,5	1.13	0
2	GOL	E	401	-	5,5,5	0.99	0	5,5,5	1.09	0
2	GOL	L	401	-	5,5,5	0.75	0	5,5,5	0.93	0
2	GOL	K	401	3	5,5,5	1.12	1 (20%)	5,5,5	0.79	0
2	GOL	F	401	-	5,5,5	0.96	0	5,5,5	1.16	0
2	GOL	G	401	-	5,5,5	0.97	0	5,5,5	0.66	0
2	GOL	D	401	-	5,5,5	1.05	0	5,5,5	1.10	0
2	GOL	I	401	-	5,5,5	1.12	0	5,5,5	1.44	1 (20%)
2	GOL	B	401	-	5,5,5	0.89	0	5,5,5	1.15	1 (20%)
2	GOL	J	401	-	5,5,5	1.10	0	5,5,5	1.07	0
2	GOL	H	403	-	5,5,5	0.56	0	5,5,5	0.32	0
2	GOL	A	401	-	5,5,5	1.06	0	5,5,5	1.08	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
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	F	402	-	-	4/4/4/4	-
2	GOL	E	401	-	-	4/4/4/4	-
2	GOL	L	401	-	-	2/4/4/4	-
2	GOL	K	401	3	-	3/4/4/4	-
2	GOL	F	401	-	-	4/4/4/4	-
2	GOL	G	401	-	-	3/4/4/4	-
2	GOL	D	401	-	-	4/4/4/4	-
2	GOL	I	401	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	401	-	-	4/4/4/4	-
2	GOL	J	401	-	-	3/4/4/4	-
2	GOL	H	403	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	GOL	C3-C2	2.16	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	401	GOL	C3-C2-C1	-2.38	102.45	111.70
2	B	401	GOL	C3-C2-C1	-2.03	103.81	111.70

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	GOL	O1-C1-C2-O2
2	G	401	GOL	O1-C1-C2-C3
2	J	401	GOL	C1-C2-C3-O3
2	F	401	GOL	C1-C2-C3-O3
2	F	402	GOL	C1-C2-C3-O3
2	C	401	GOL	O1-C1-C2-C3
2	H	403	GOL	O2-C2-C3-O3
2	F	402	GOL	O2-C2-C3-O3
2	L	401	GOL	O1-C1-C2-C3
2	K	401	GOL	O1-C1-C2-C3
2	K	401	GOL	C1-C2-C3-O3
2	H	403	GOL	C1-C2-C3-O3
2	F	401	GOL	O1-C1-C2-C3
2	F	402	GOL	O1-C1-C2-C3
2	E	401	GOL	O1-C1-C2-C3
2	E	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	F	401	GOL	O1-C1-C2-O2
2	E	401	GOL	O2-C2-C3-O3
2	K	401	GOL	O1-C1-C2-O2
2	J	401	GOL	O2-C2-C3-O3
2	F	401	GOL	O2-C2-C3-O3
2	C	401	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
2	B	401	GOL	O1-C1-C2-O2
2	L	401	GOL	O1-C1-C2-O2
2	F	402	GOL	O1-C1-C2-O2
2	E	401	GOL	O1-C1-C2-O2
2	G	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O2-C2-C3-O3
2	J	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	289/306 (94%)	-0.61	1 (0%) 90 91	30, 42, 57, 92	0
1	B	288/306 (94%)	-0.63	0 100 100	31, 43, 63, 117	0
1	C	287/306 (93%)	-0.43	0 100 100	34, 49, 68, 90	0
1	D	288/306 (94%)	-0.31	0 100 100	35, 52, 76, 110	0
1	E	288/306 (94%)	-0.44	1 (0%) 90 91	33, 50, 73, 100	0
1	F	291/306 (95%)	-0.53	0 100 100	32, 46, 67, 100	0
1	G	288/306 (94%)	-0.13	0 100 100	41, 67, 95, 119	0
1	H	286/306 (93%)	0.25	10 (3%) 47 53	30, 75, 108, 126	0
1	I	285/306 (93%)	0.01	1 (0%) 89 90	42, 67, 91, 113	0
1	J	288/306 (94%)	-0.49	0 100 100	32, 45, 69, 98	0
1	K	287/306 (93%)	0.12	4 (1%) 73 77	40, 76, 109, 142	0
1	L	287/306 (93%)	-0.12	0 100 100	39, 64, 93, 116	0
All	All	3452/3672 (94%)	-0.28	17 (0%) 87 89	30, 54, 93, 142	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	99	ASP	6.8
1	H	272	ASN	4.3
1	H	284	GLU	4.3
1	H	295	ARG	3.7
1	E	9	ARG	3.5
1	K	296	PRO	3.2
1	H	100	VAL	2.8
1	K	20	TYR	2.7
1	H	60	GLN	2.7
1	K	274	TRP	2.7
1	H	59	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	90	LEU	2.5
1	K	10	ASP	2.5
1	I	93	VAL	2.4
1	H	43	ILE	2.3
1	H	95	PHE	2.3
1	A	8	PRO	2.2

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, 95^{th} 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
2	GOL	H	403	6/6	0.25	0.29	30,30,30,30	0
2	GOL	E	401	6/6	0.80	0.15	47,68,78,85	0
2	GOL	L	401	6/6	0.82	0.13	61,74,85,91	0
2	GOL	B	401	6/6	0.82	0.16	48,62,74,81	0
2	GOL	F	402	6/6	0.83	0.12	53,76,88,95	0
2	GOL	G	401	6/6	0.83	0.14	53,73,89,89	0
2	GOL	J	401	6/6	0.83	0.12	42,55,73,76	0
2	GOL	C	401	6/6	0.83	0.13	49,67,82,93	0
2	GOL	F	401	6/6	0.85	0.12	44,66,77,79	0
3	ZN	K	403	1/1	0.86	0.10	76,76,76,76	0
2	GOL	A	401	6/6	0.87	0.12	47,64,80,83	0
2	GOL	I	401	6/6	0.87	0.11	58,77,94,97	0
2	GOL	D	401	6/6	0.90	0.11	47,70,84,86	0
2	GOL	K	401	6/6	0.90	0.14	64,85,102,102	0
3	ZN	H	402	1/1	0.91	0.08	69,69,69,69	0
3	ZN	J	403	1/1	0.91	0.08	57,57,57,57	0
3	ZN	D	403	1/1	0.93	0.08	56,56,56,56	0

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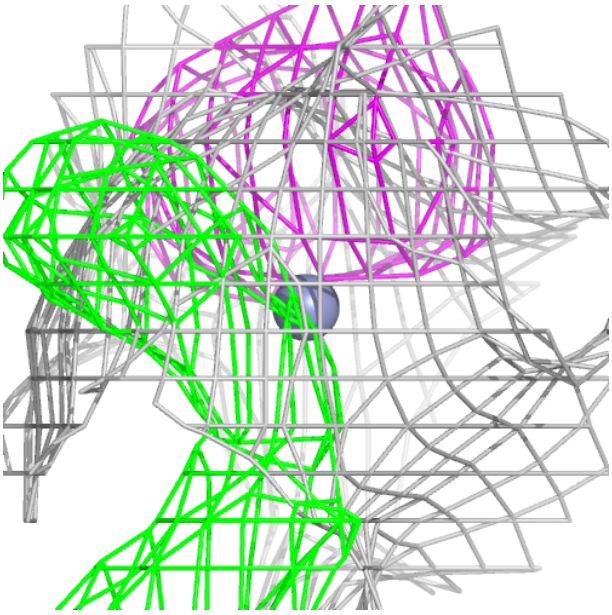
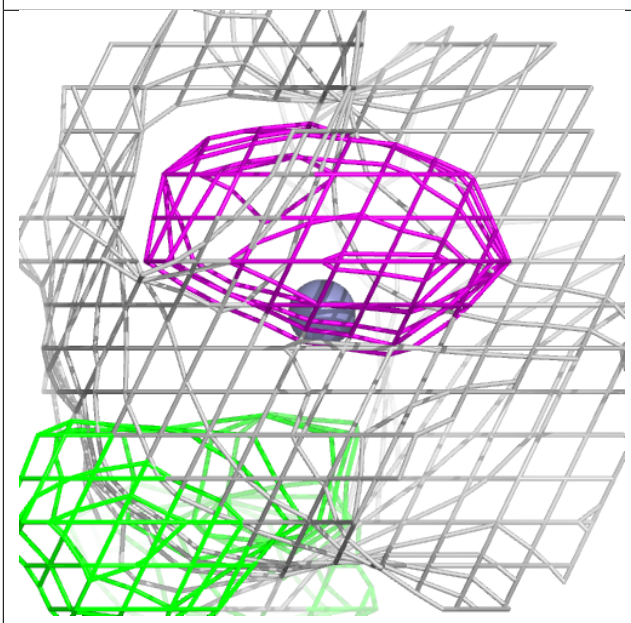
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	L	403	1/1	0.94	0.26	30,30,30,30	0
3	ZN	F	404	1/1	0.94	0.07	56,56,56,56	0
3	ZN	C	403	1/1	0.94	0.08	54,54,54,54	0
3	ZN	I	403	1/1	0.94	0.09	72,72,72,72	0
3	ZN	I	402	1/1	0.96	0.04	60,60,60,60	0
3	ZN	G	403	1/1	0.98	0.04	65,65,65,65	0
3	ZN	E	403	1/1	0.98	0.06	54,54,54,54	0
3	ZN	H	401	1/1	0.98	0.05	66,66,66,66	0
3	ZN	K	402	1/1	0.98	0.04	66,66,66,66	0
3	ZN	E	402	1/1	0.99	0.02	45,45,45,45	0
3	ZN	G	402	1/1	0.99	0.05	58,58,58,58	0
3	ZN	A	402	1/1	0.99	0.02	42,42,42,42	0
3	ZN	A	403	1/1	0.99	0.03	52,52,52,52	0
3	ZN	B	402	1/1	0.99	0.02	37,37,37,37	0
3	ZN	C	402	1/1	0.99	0.02	48,48,48,48	0
3	ZN	F	403	1/1	0.99	0.09	58,58,58,58	0
3	ZN	D	402	1/1	0.99	0.03	46,46,46,46	0
3	ZN	L	402	1/1	0.99	0.03	54,54,54,54	0
3	ZN	J	402	1/1	1.00	0.02	46,46,46,46	0
3	ZN	B	403	1/1	1.00	0.07	42,42,42,42	0

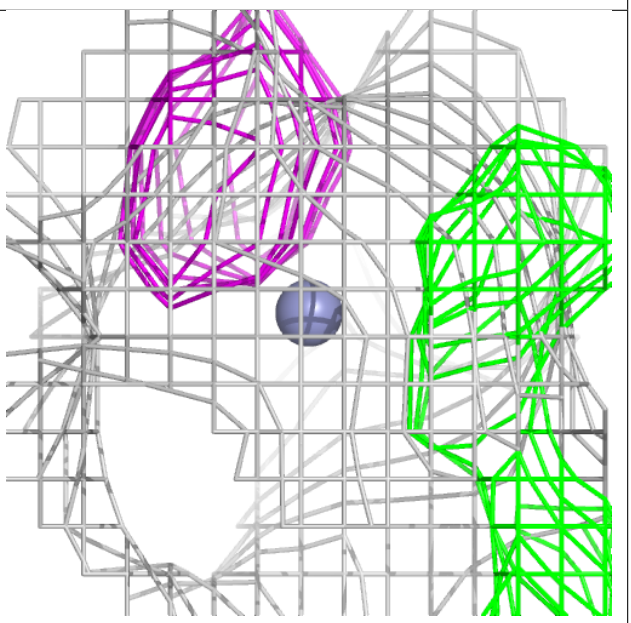
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN K 403:

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

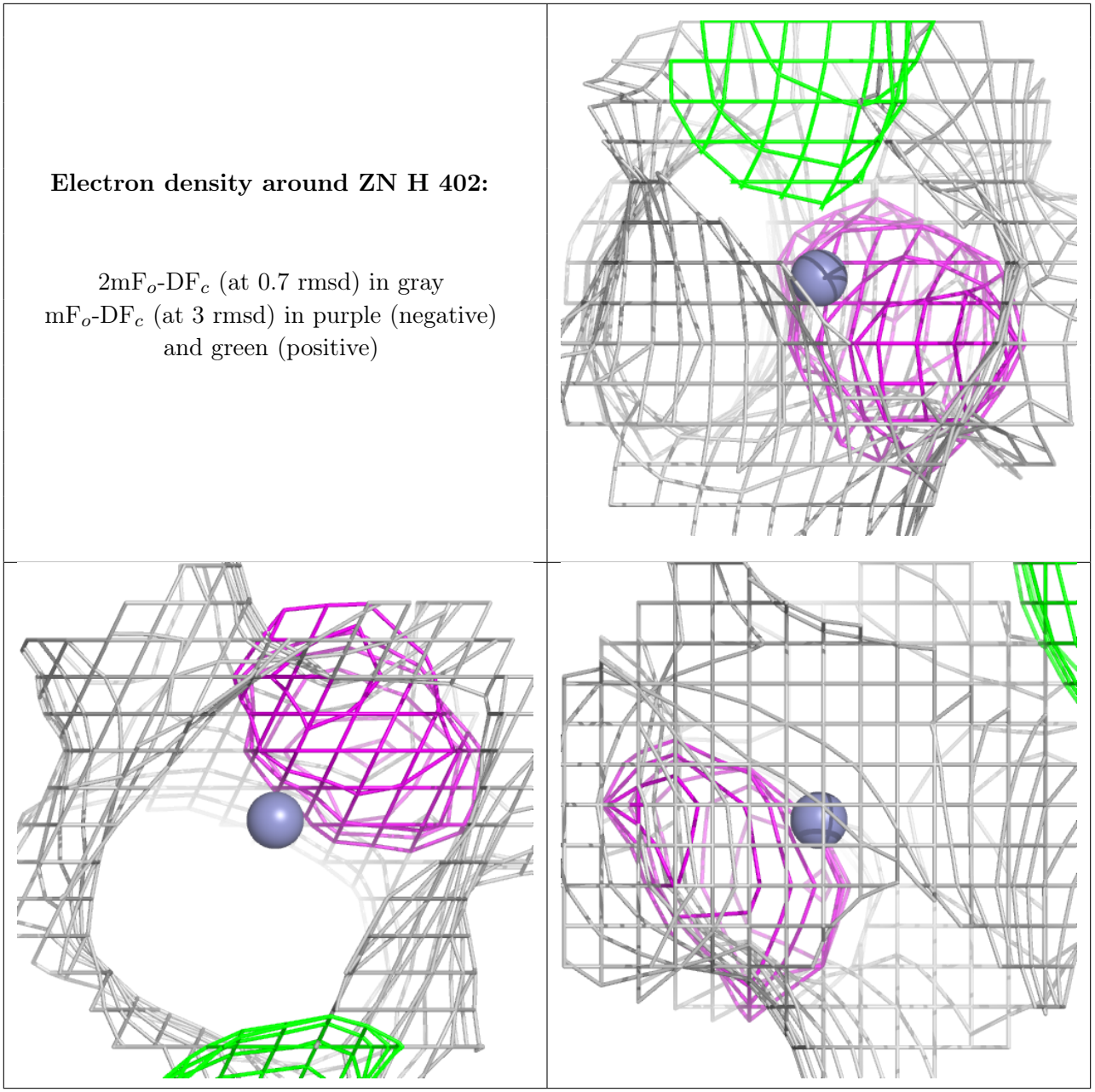






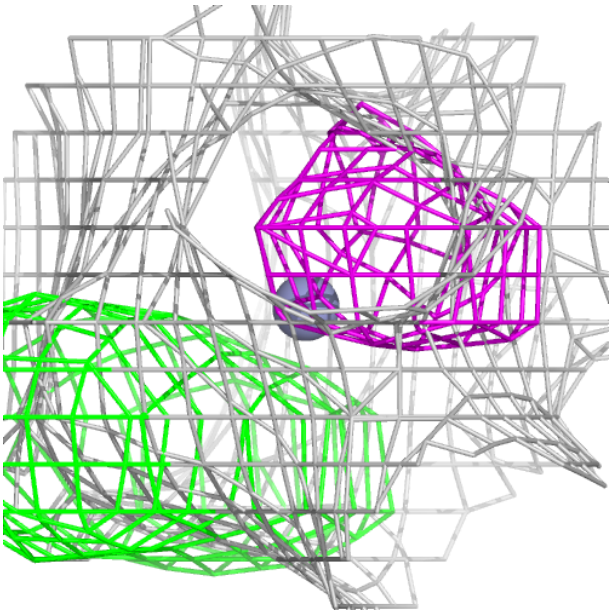
Electron density around ZN H 402:

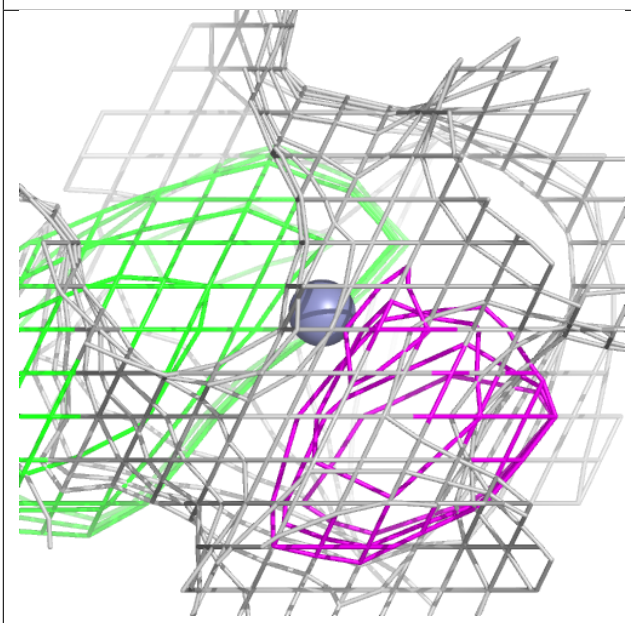
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

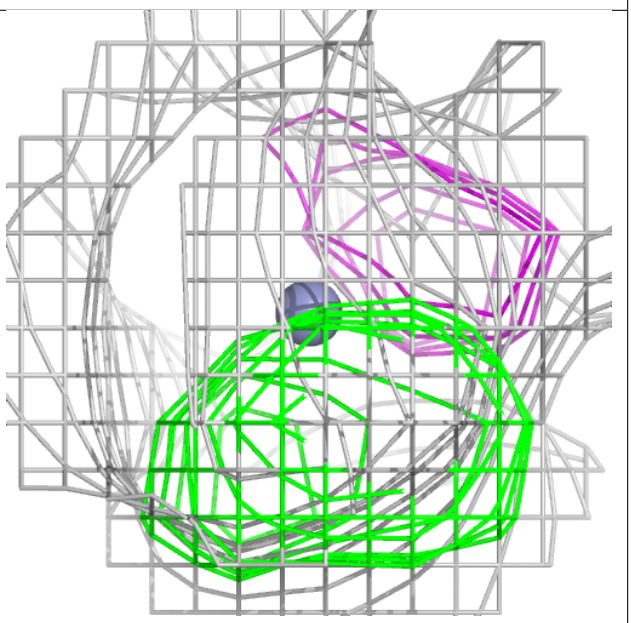


Electron density around ZN J 403:

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

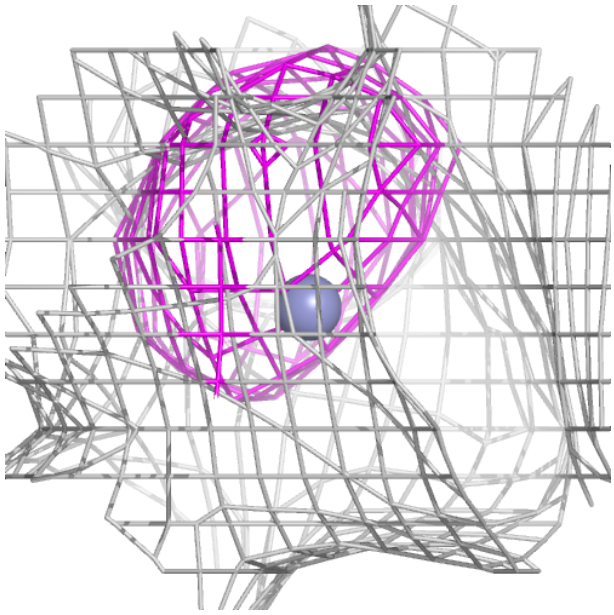


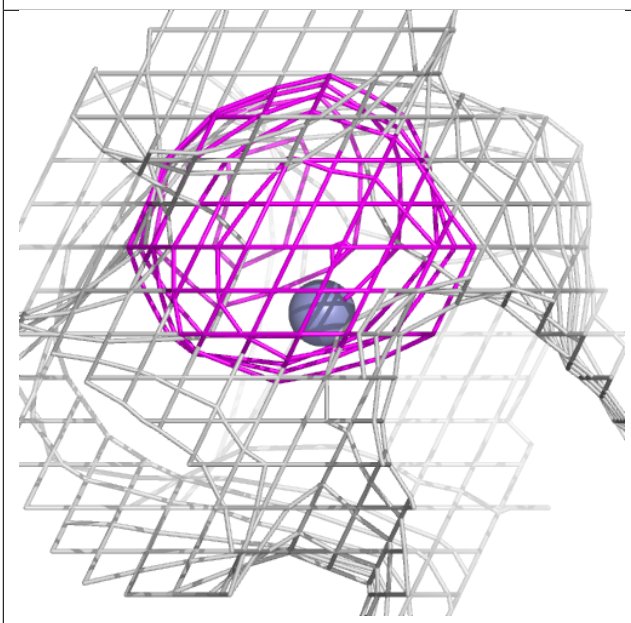


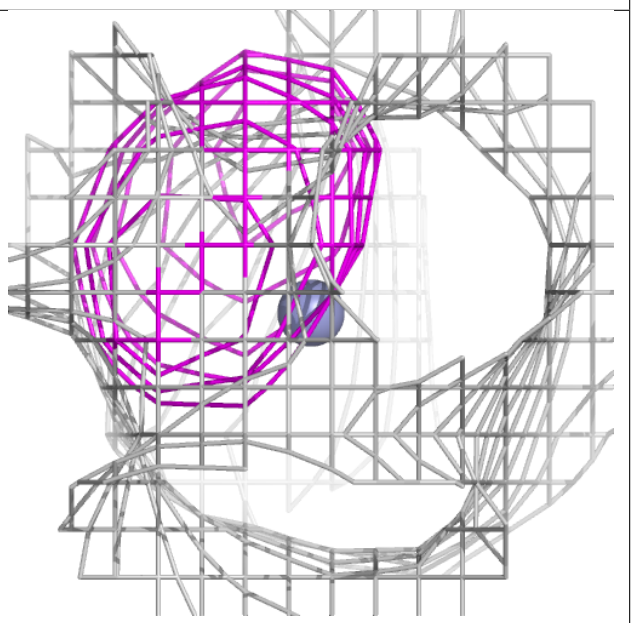


Electron density around ZN D 403:

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

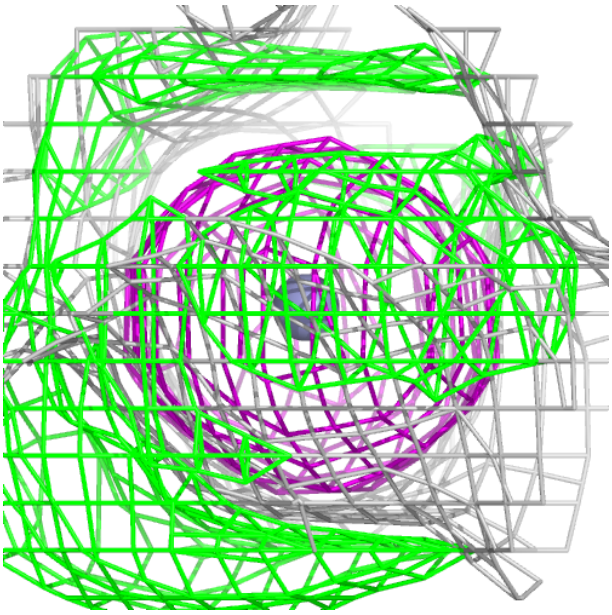


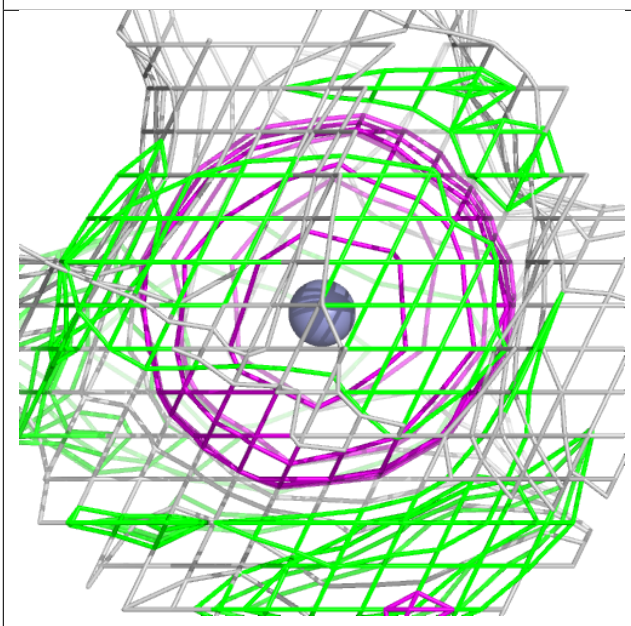


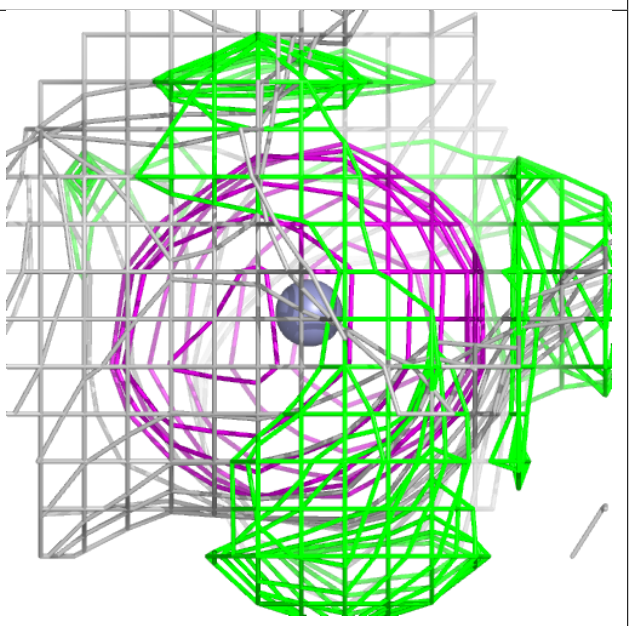


Electron density around ZN L 403:

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

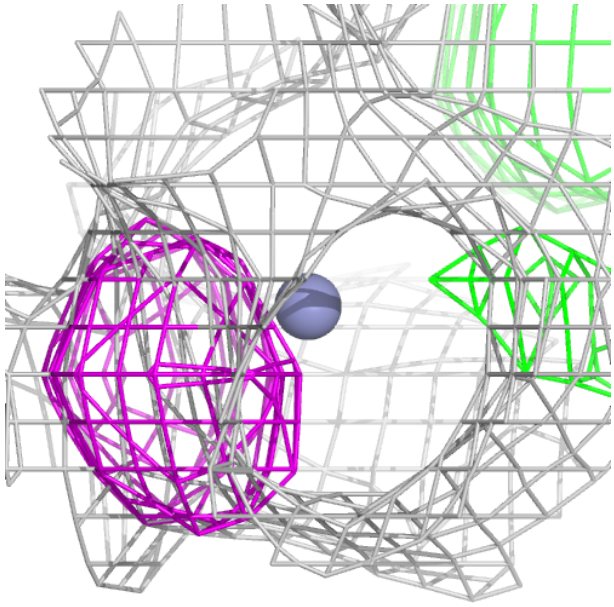


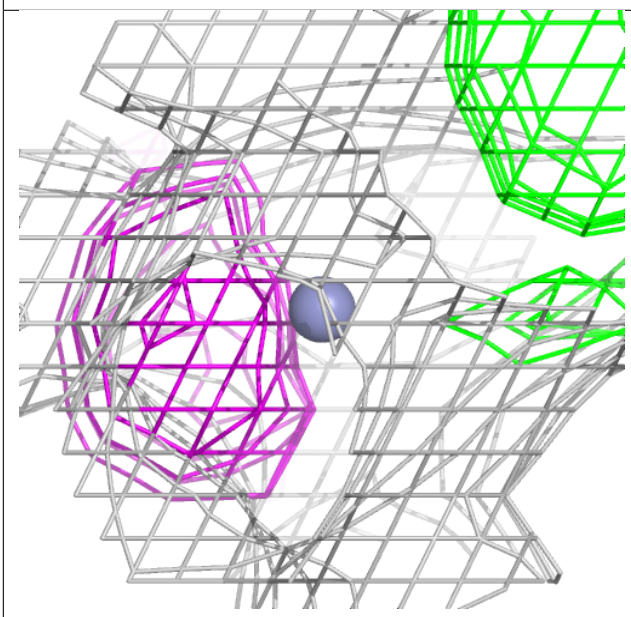


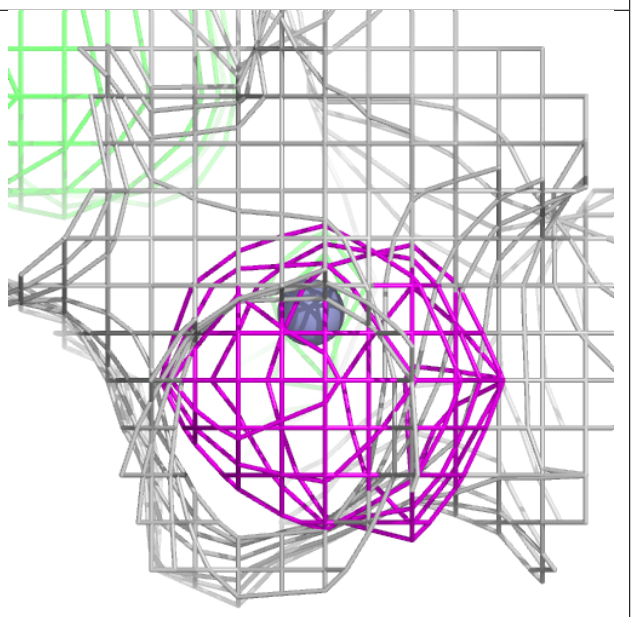


Electron density around ZN F 404:

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

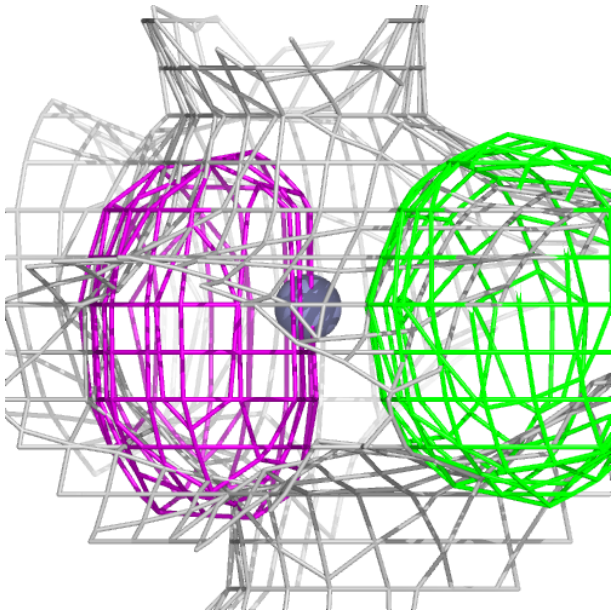


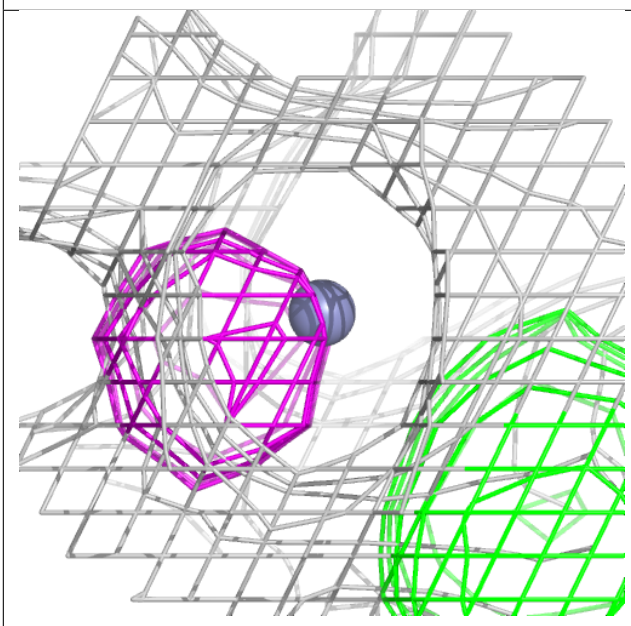


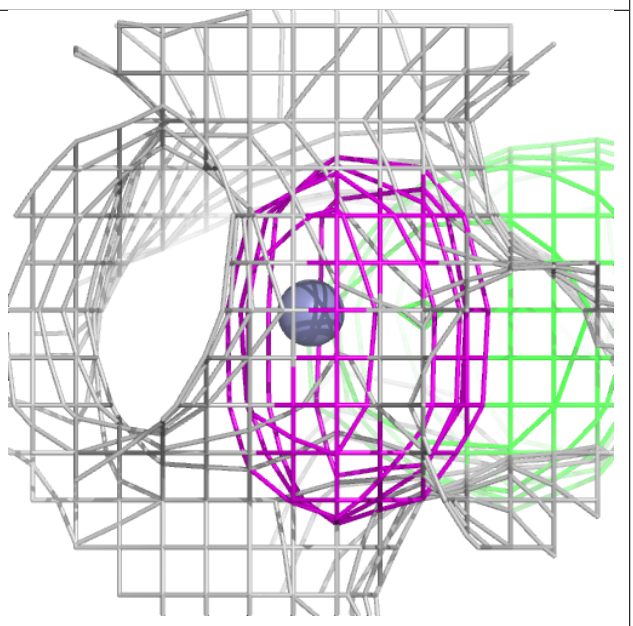


Electron density around ZN C 403:

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

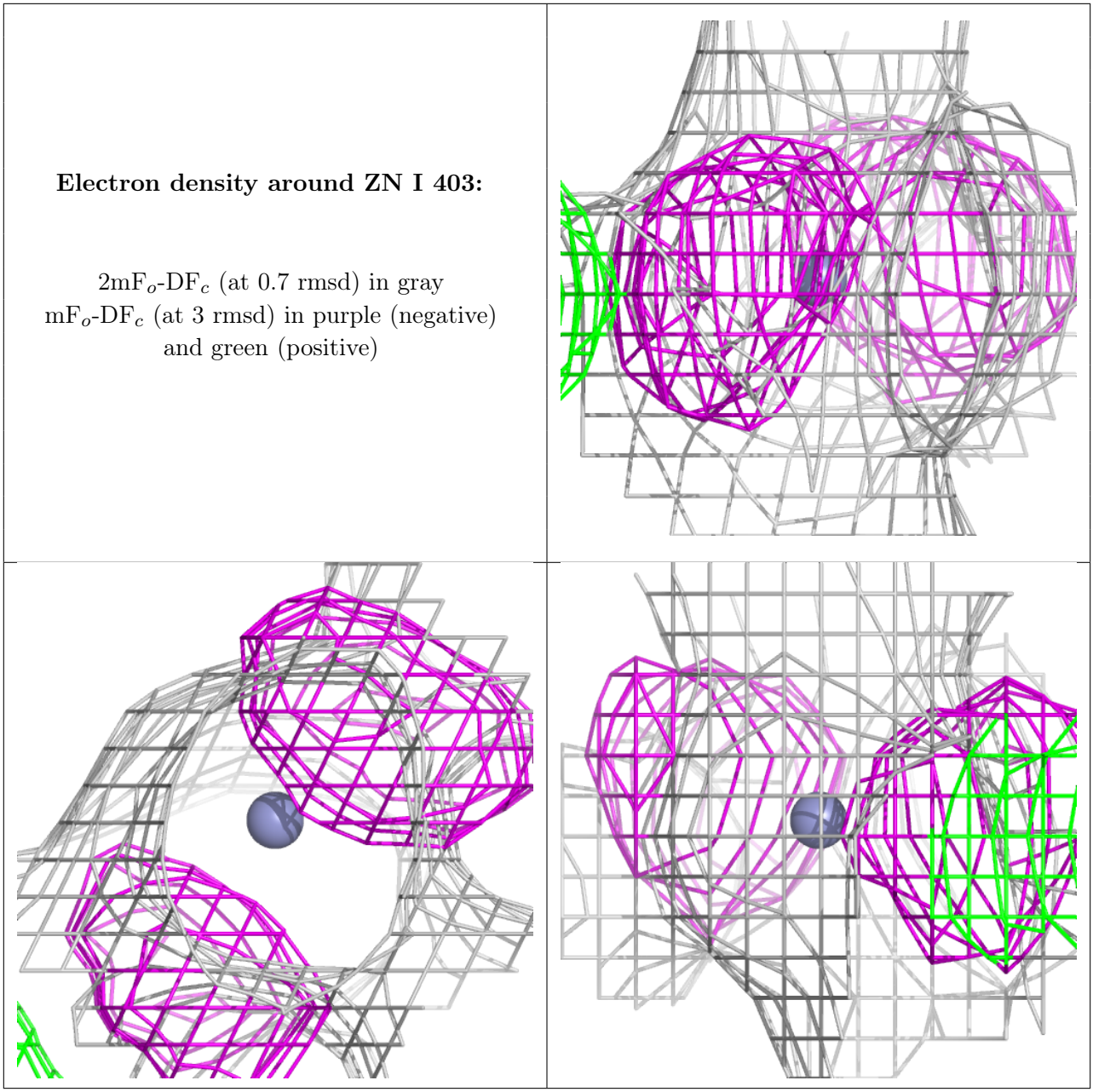






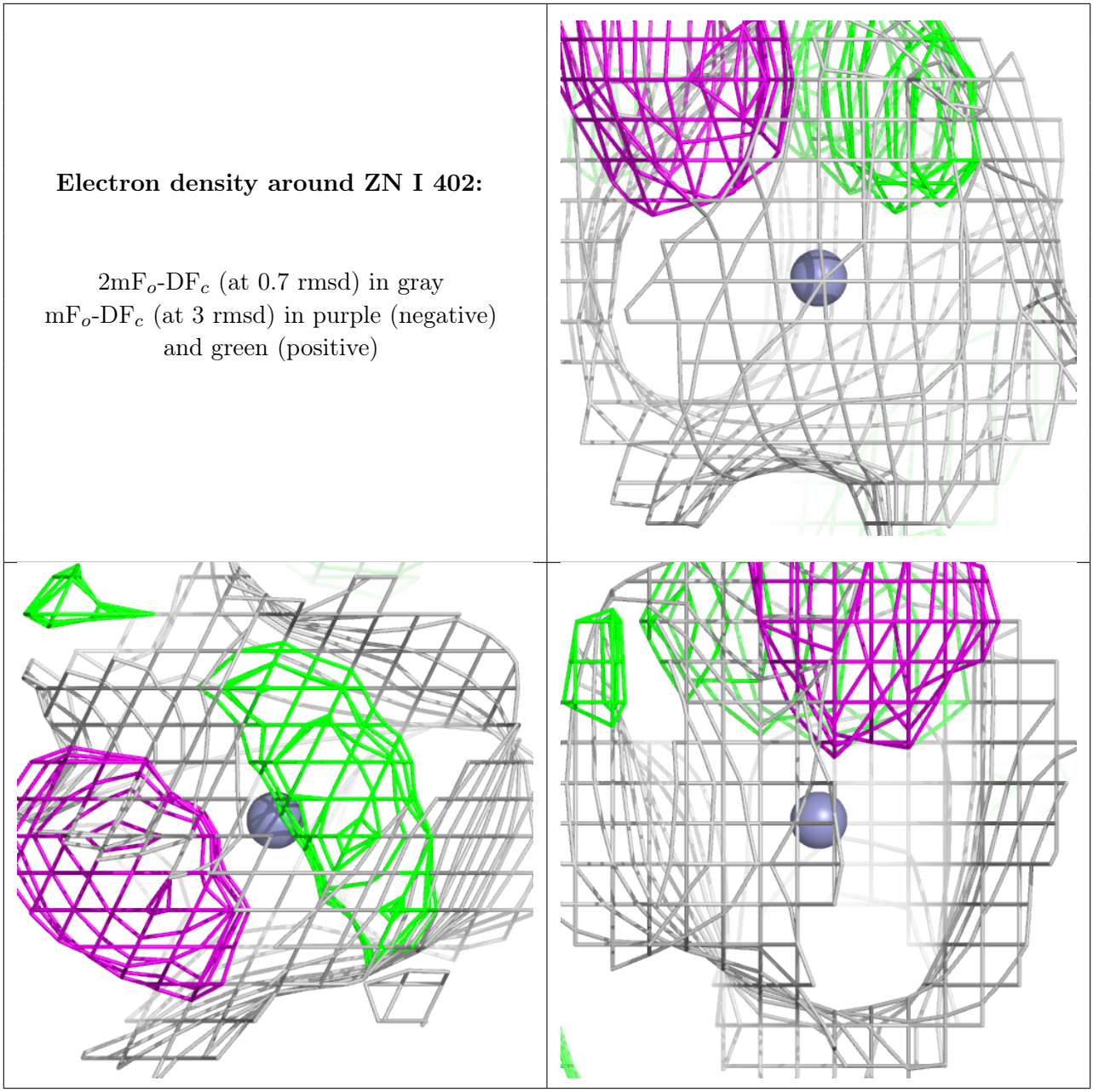
Electron density around ZN I 403:

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



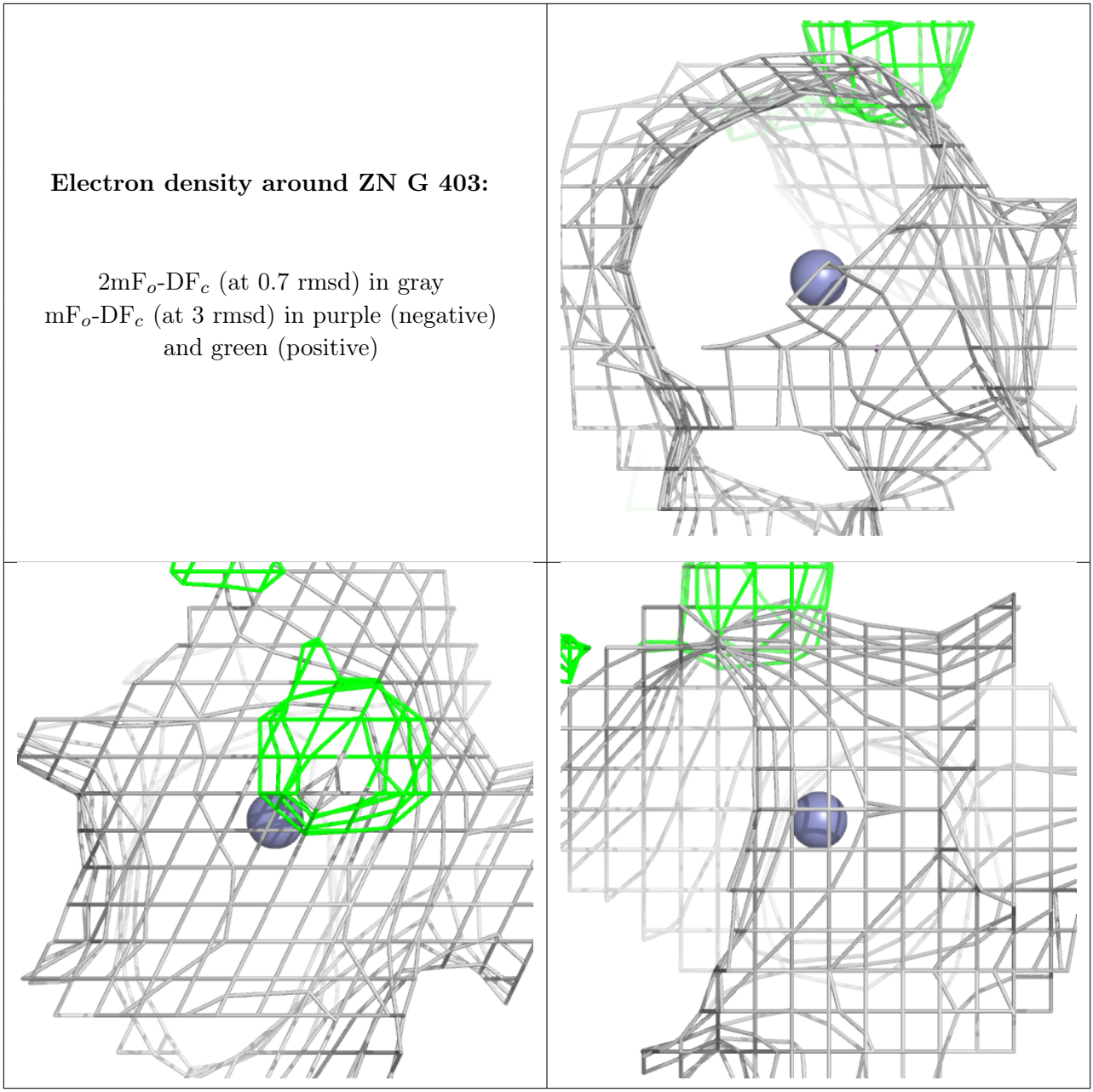
Electron density around ZN I 402:

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



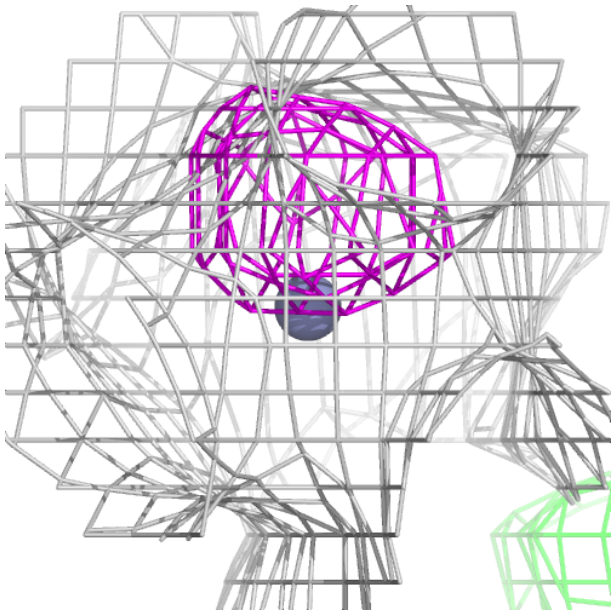
Electron density around ZN G 403:

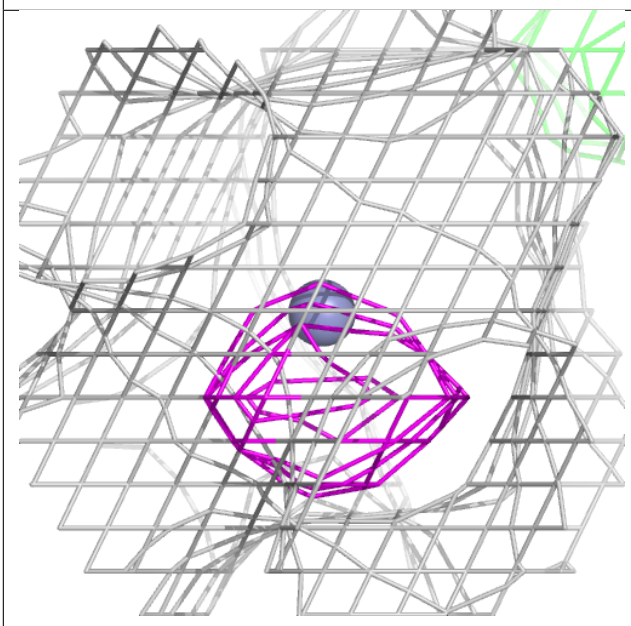
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

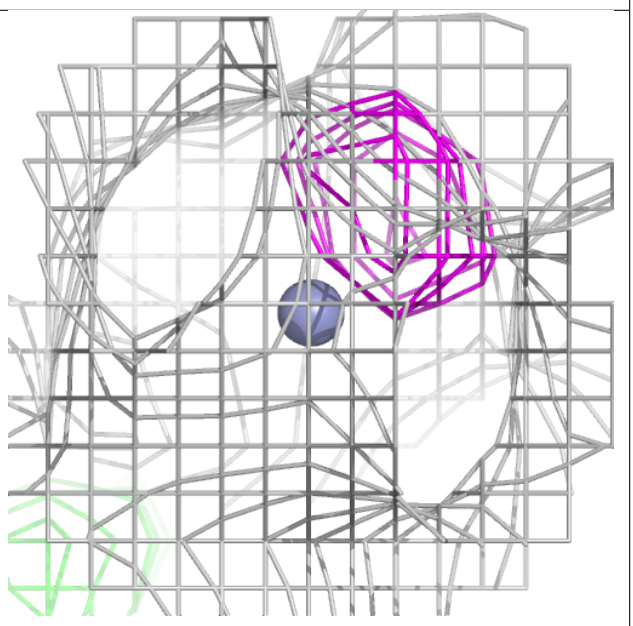


Electron density around ZN E 403:

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

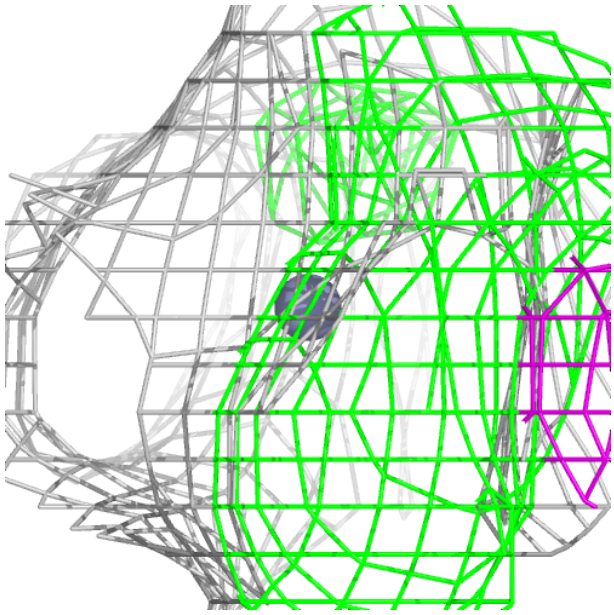


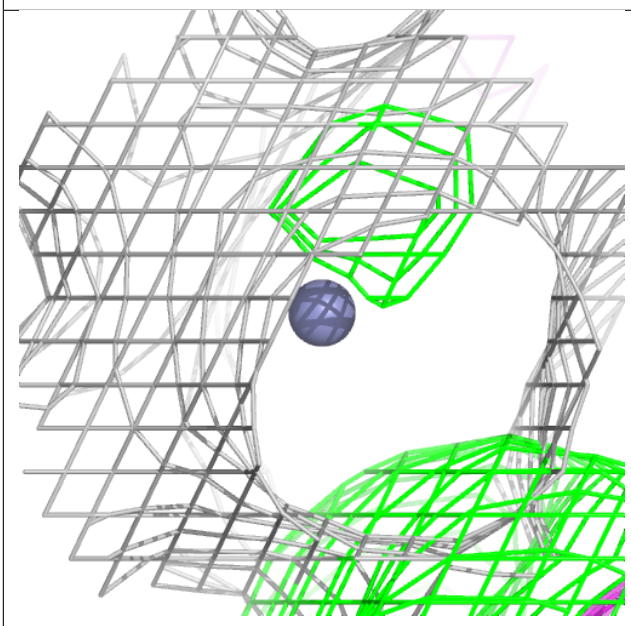


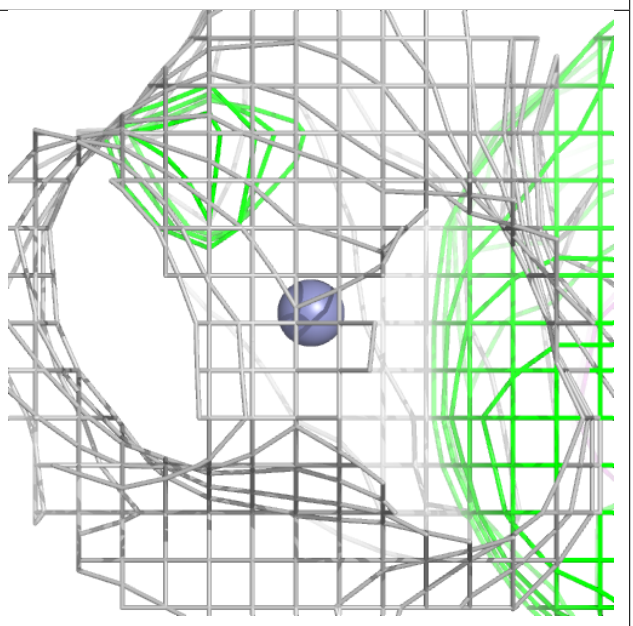


Electron density around ZN H 401:

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

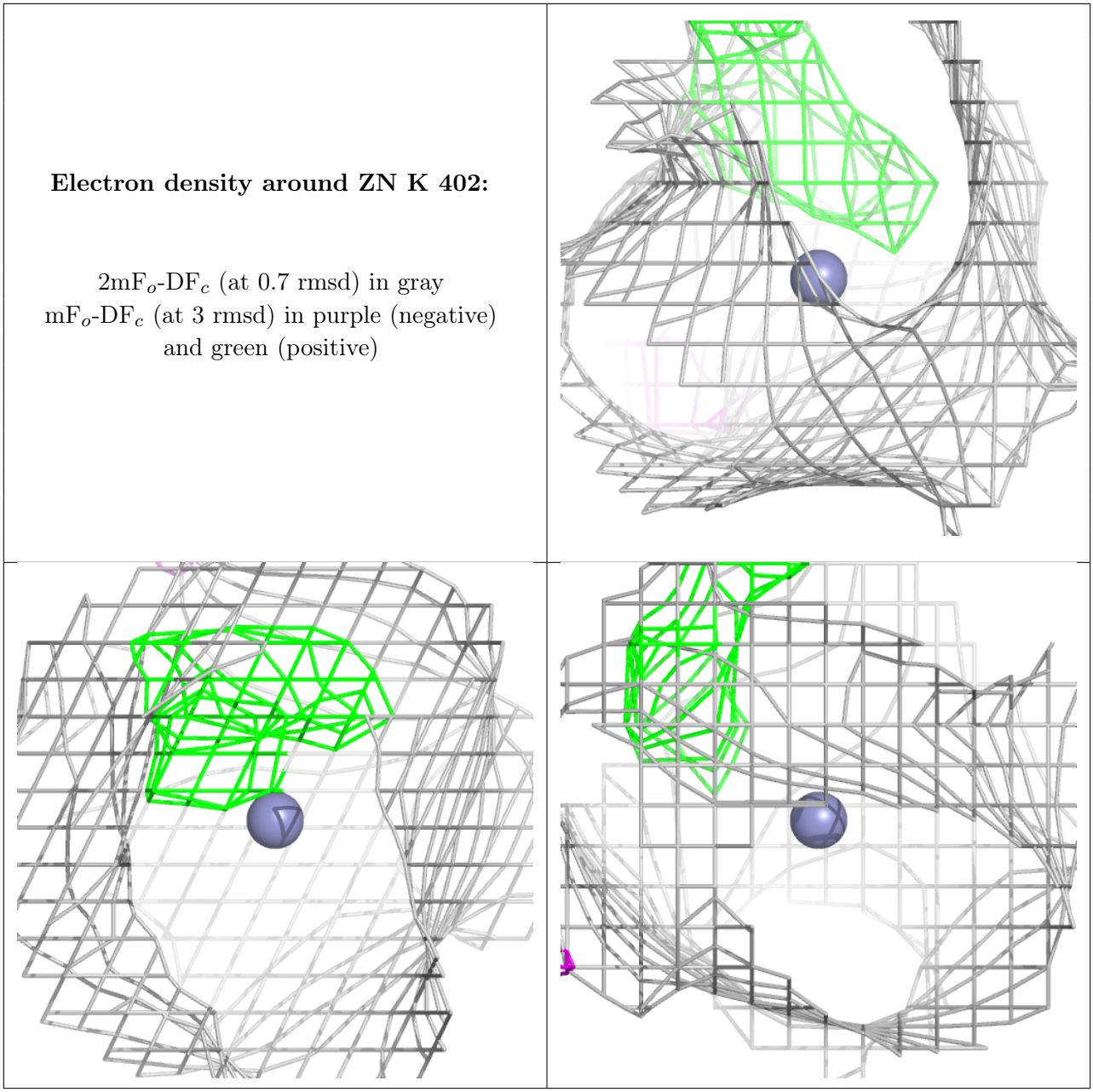






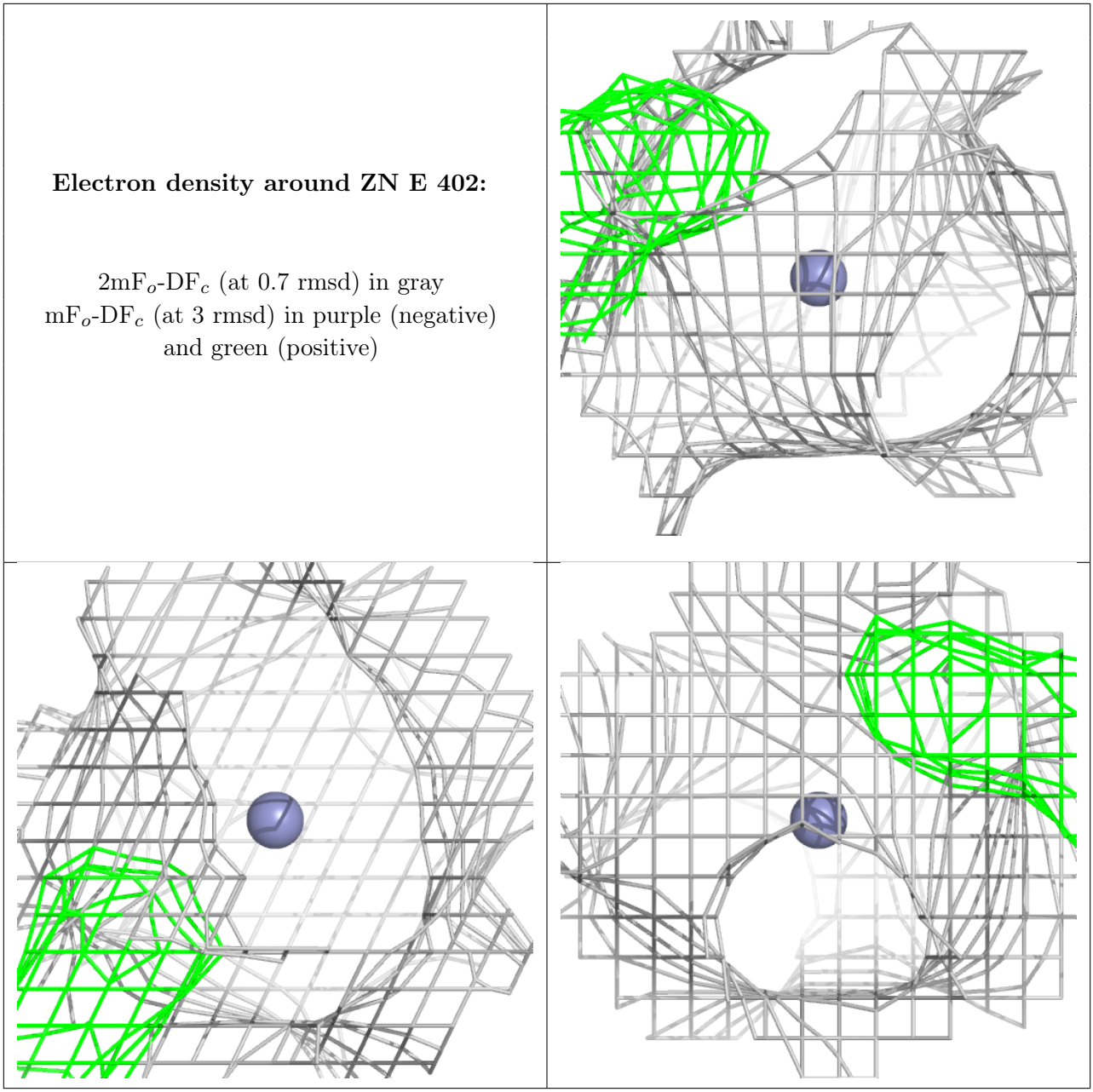
Electron density around ZN K 402:

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



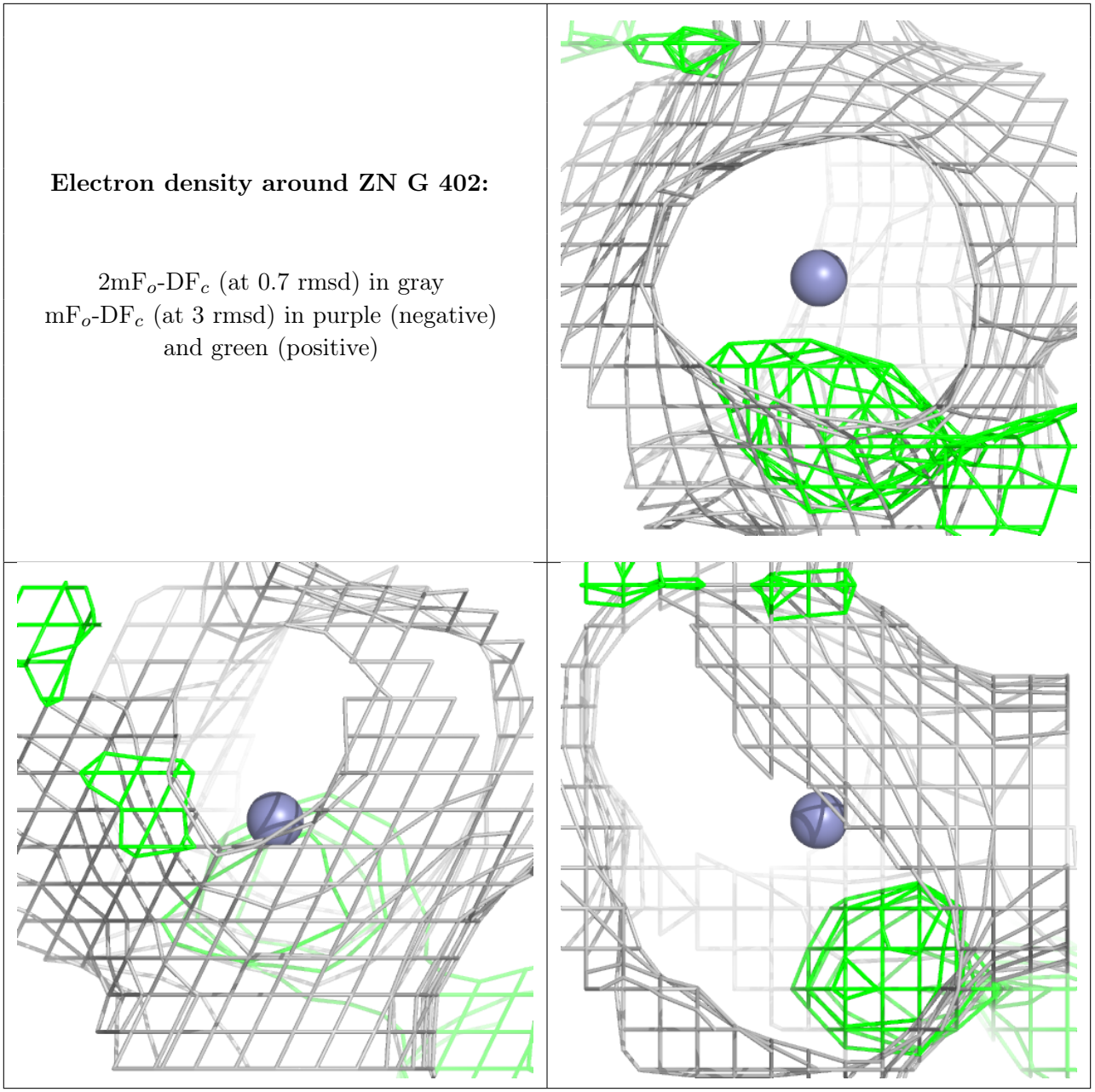
Electron density around ZN E 402:

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



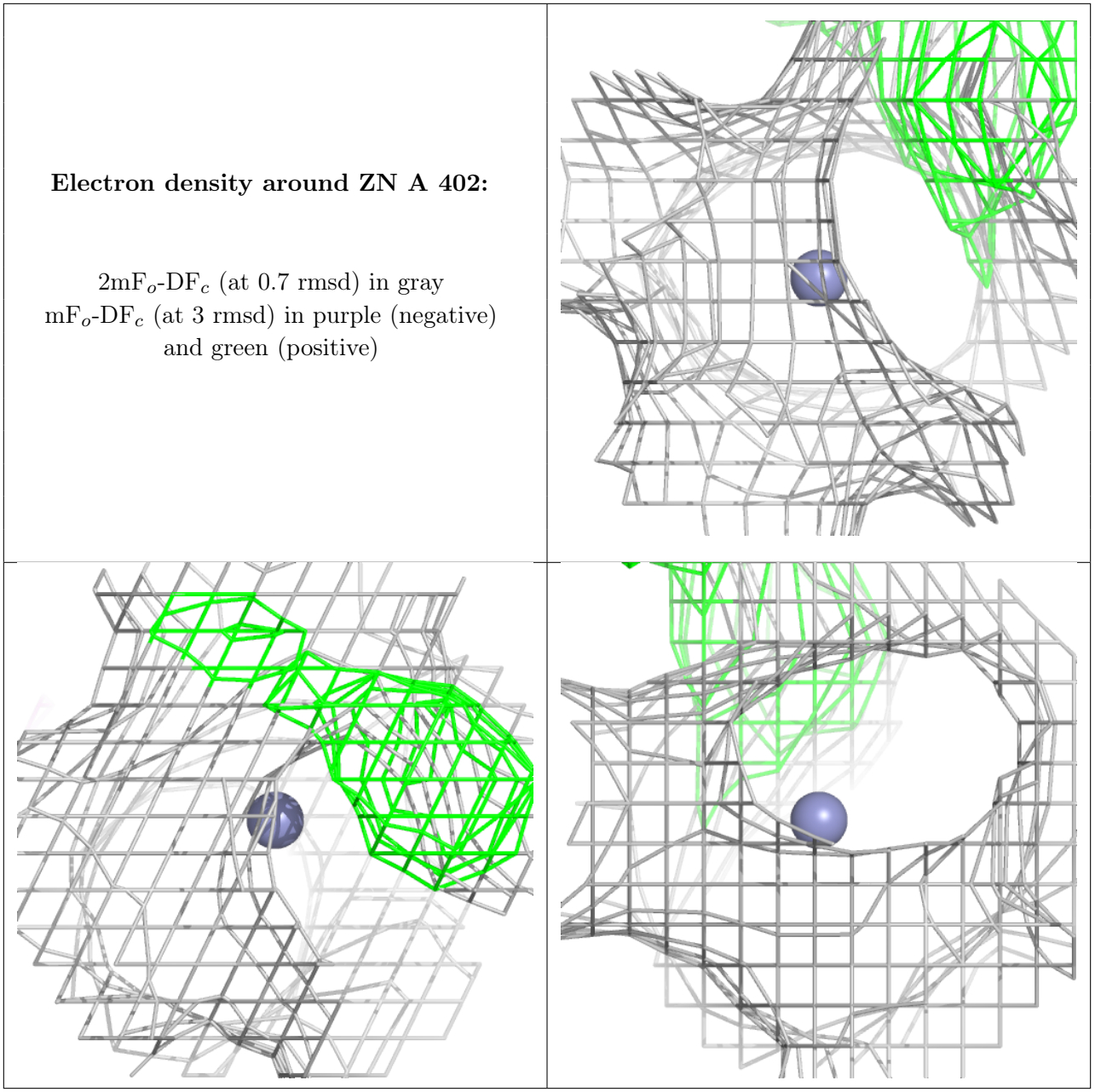
Electron density around ZN G 402:

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



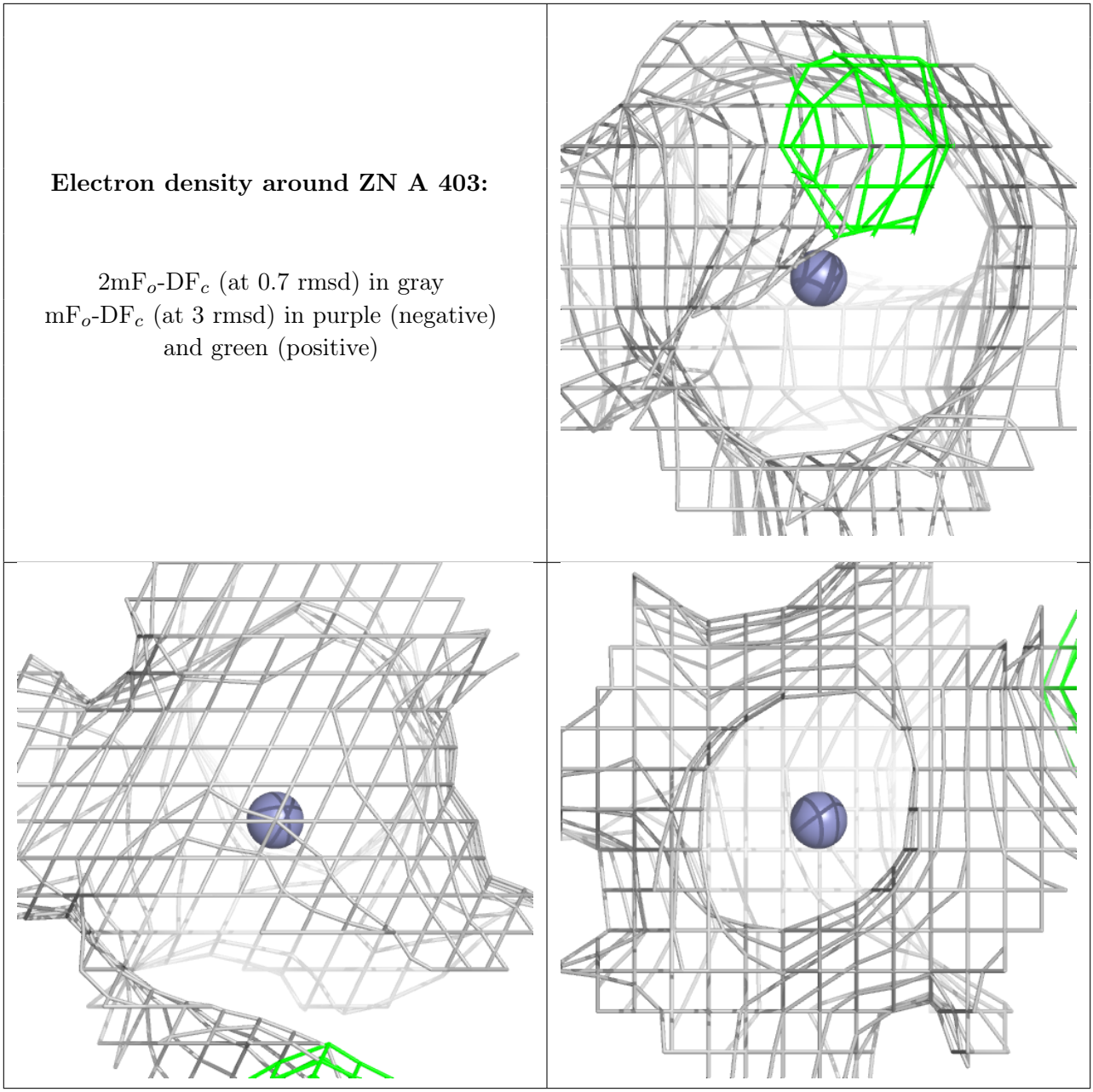
Electron density around ZN A 402:

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



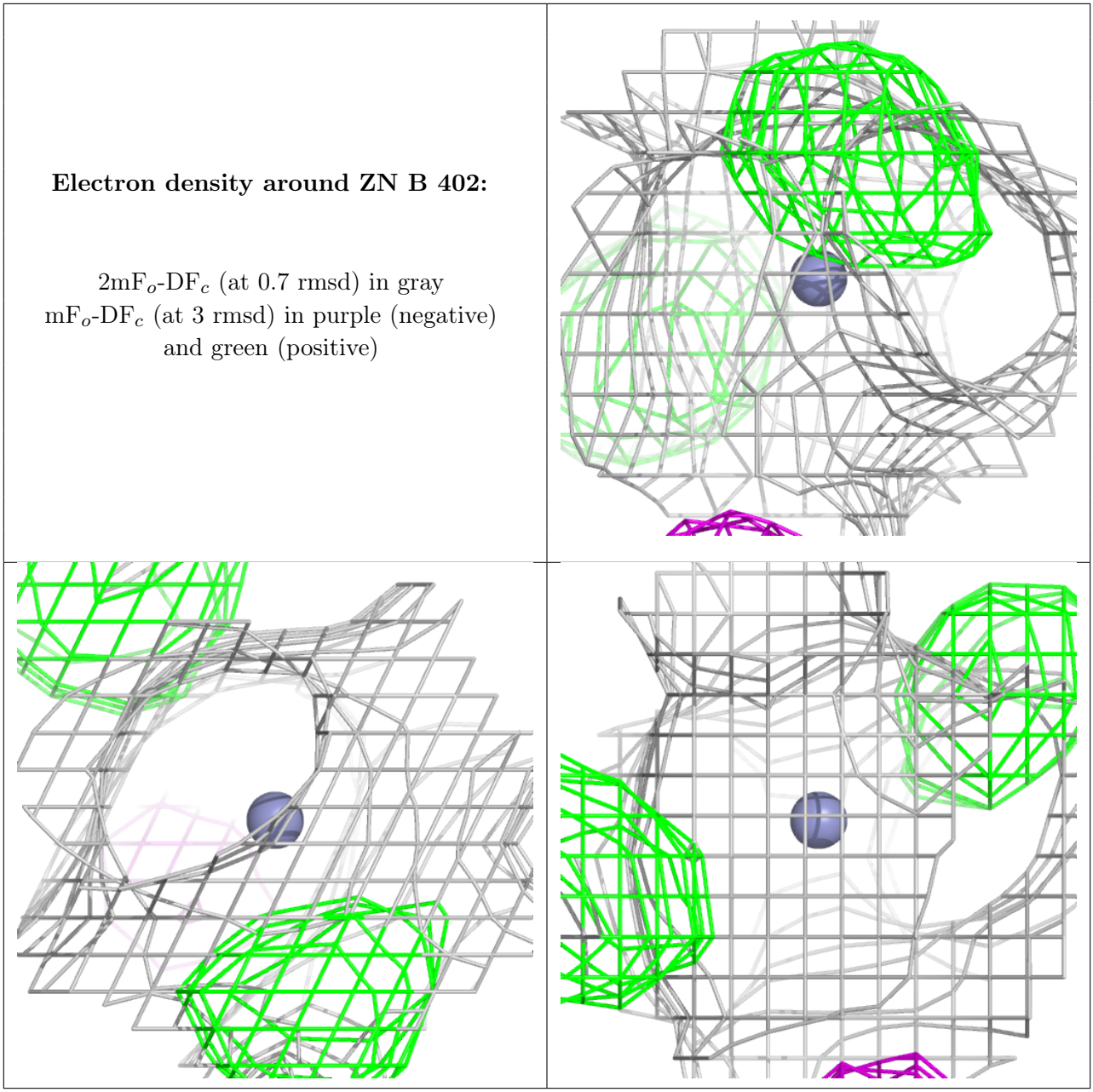
Electron density around ZN A 403:

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



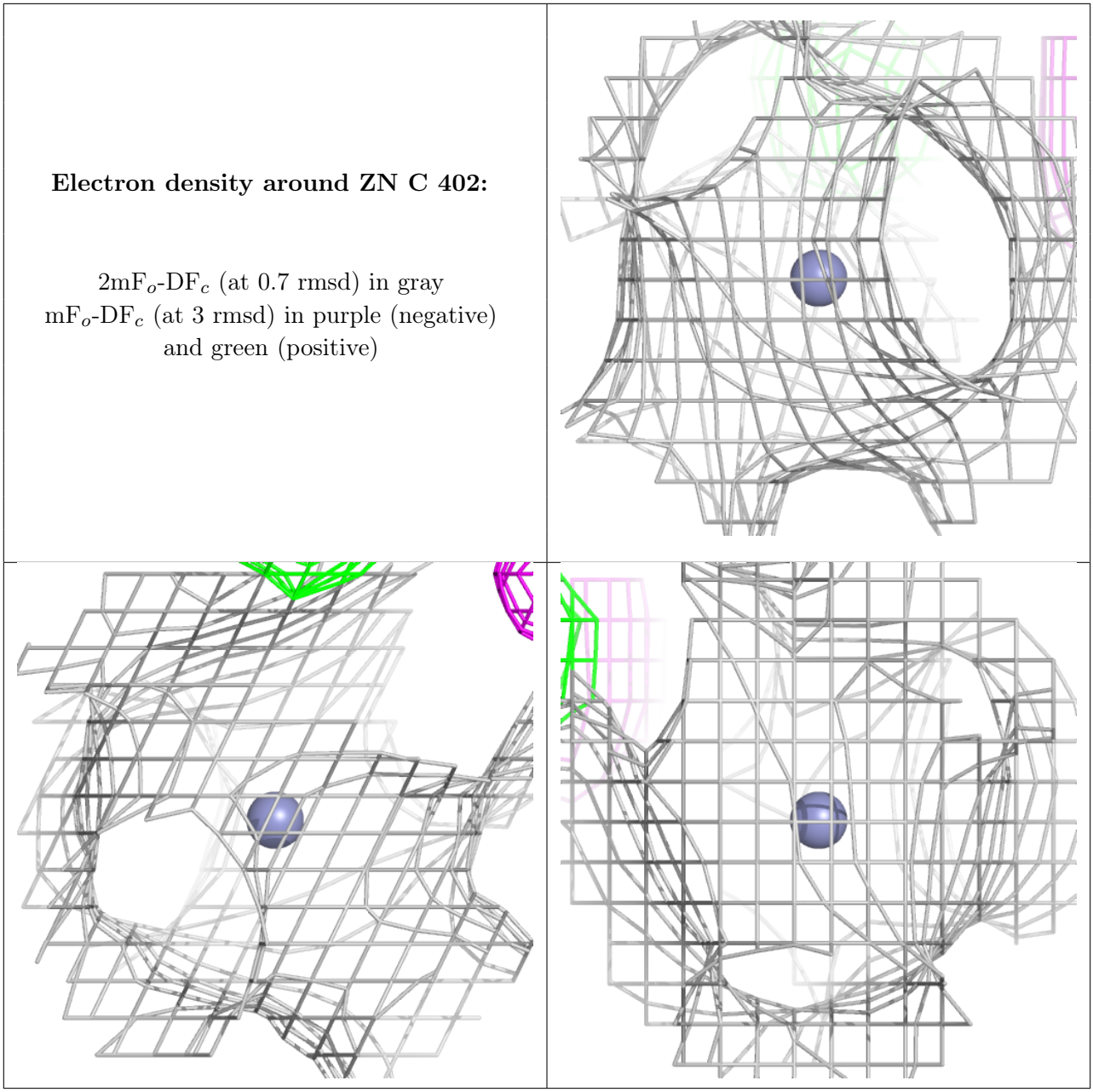
Electron density around ZN B 402:

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



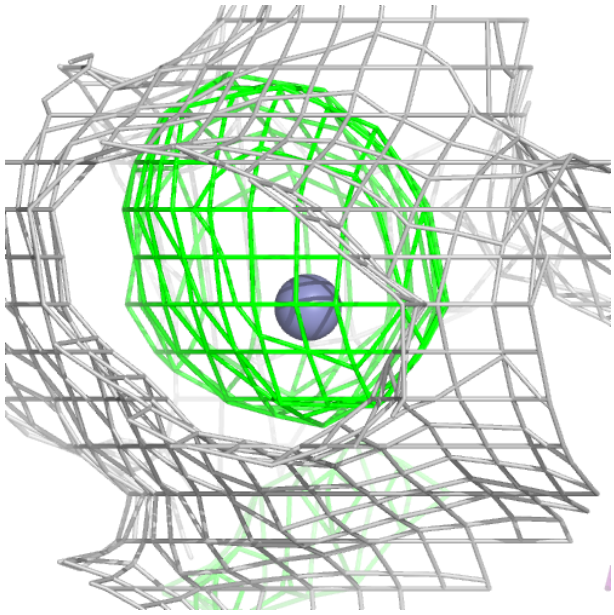
Electron density around ZN C 402:

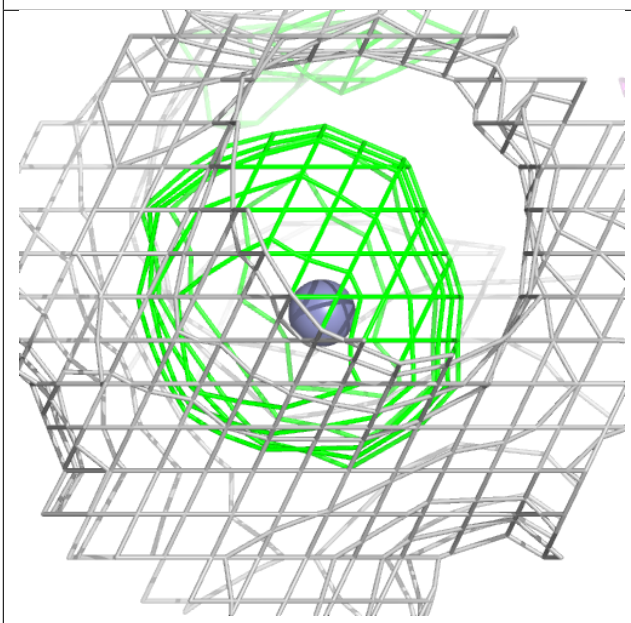
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

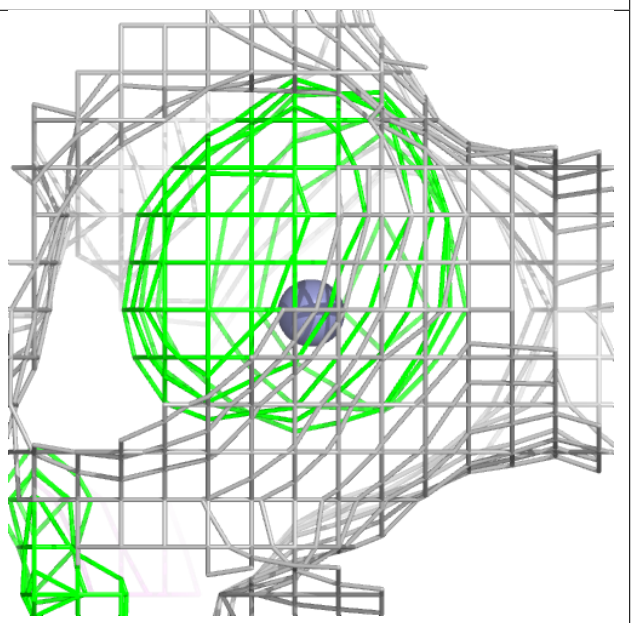


Electron density around ZN F 403:

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

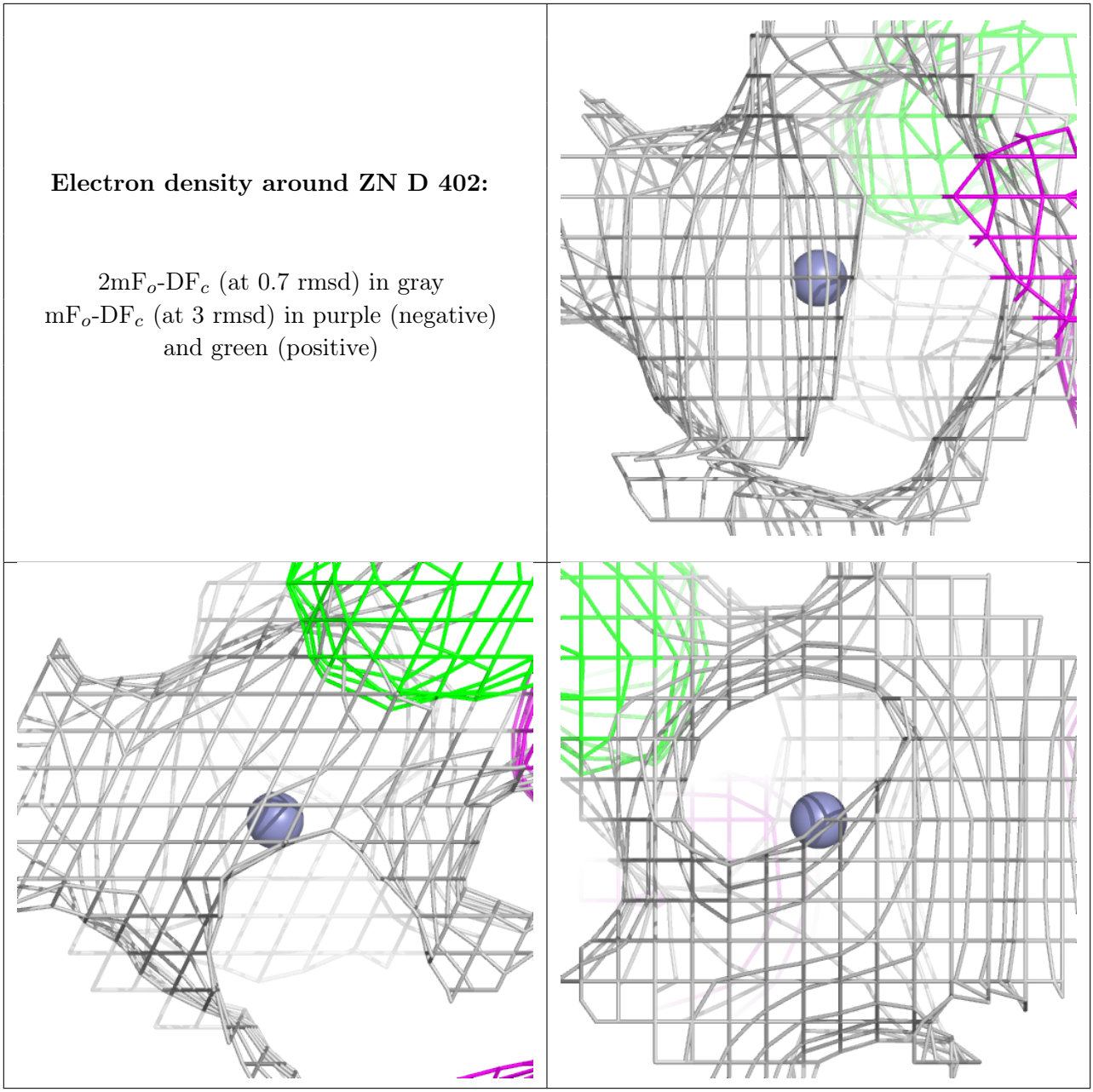






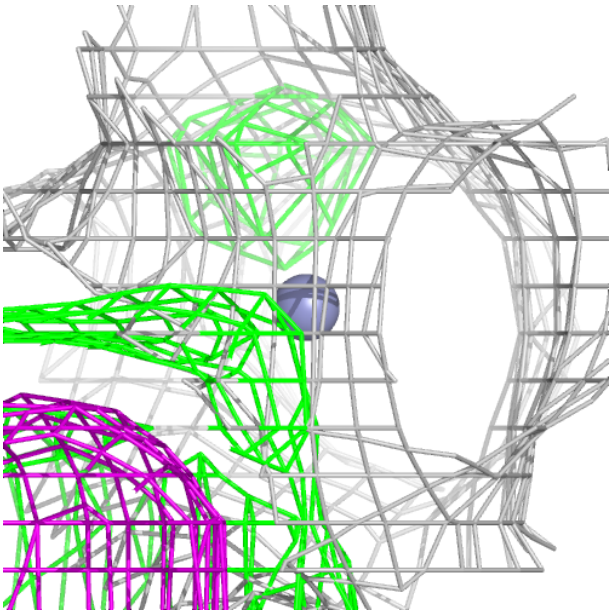
Electron density around ZN D 402:

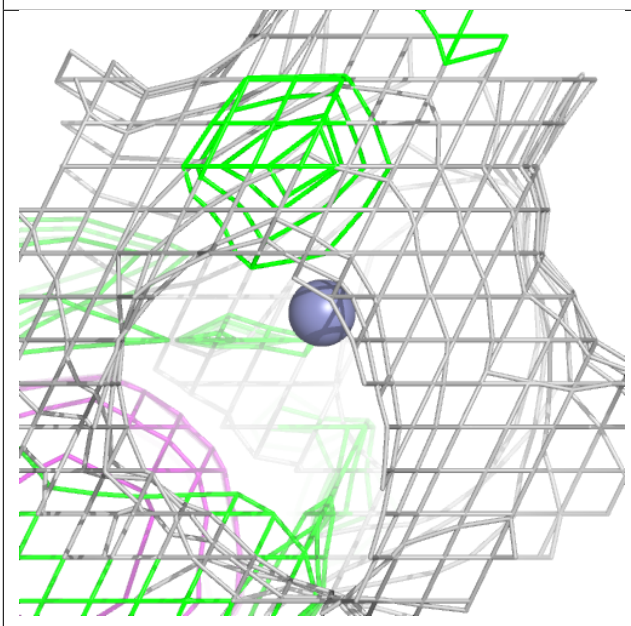
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

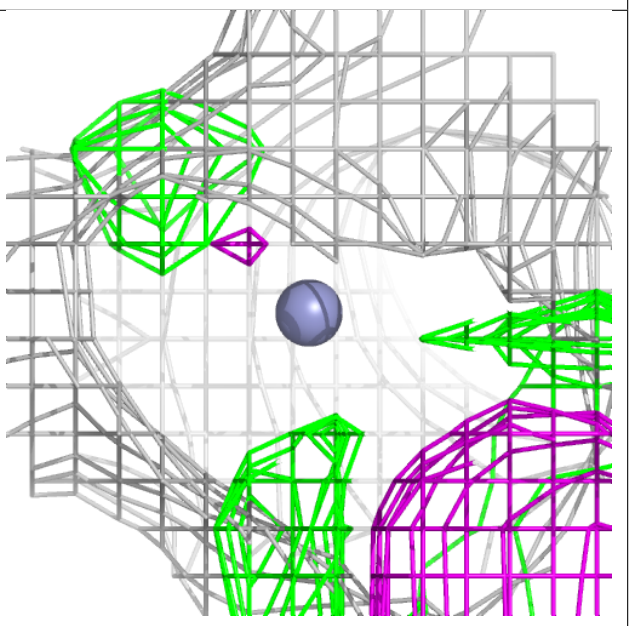


Electron density around ZN L 402:

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

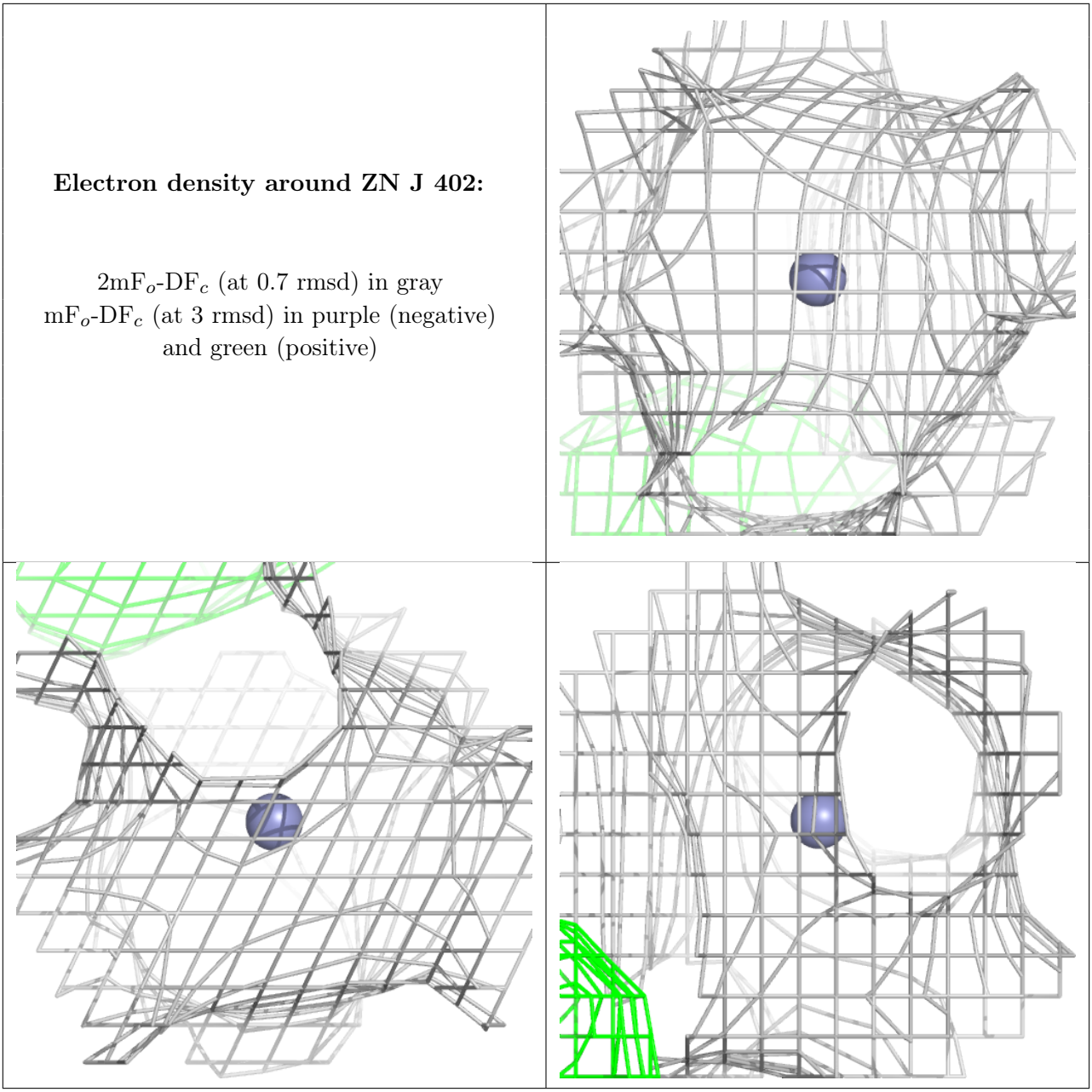






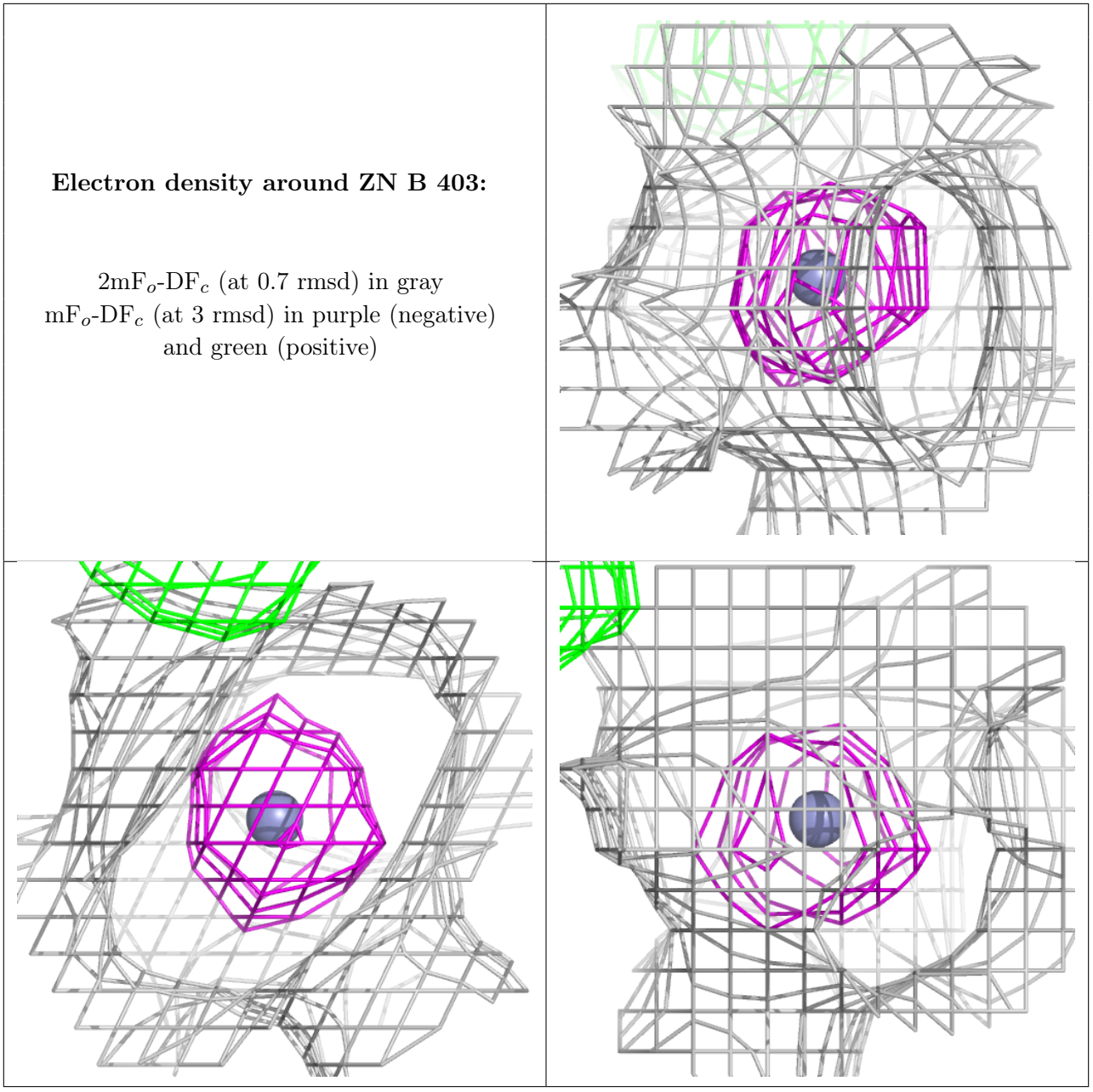
Electron density around ZN J 402:

$2mF_o$-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 403:

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



6.5 Other polymers

There are no such residues in this entry.