Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2024 – 02:02 PM EST

PDB ID	:	7JYY
Title	:	Crystal Structure of SARS-CoV-2 Nsp16/10 Heterodimer in Complex with (m7GpppA)pUpUpApApA (Cap-0) and S-Adenosylmethionine (SAM).
Authors	:	Minasov, G.; Shuvalova, L.; Rosas-Lemus, M.; Kiryukhina, O.; Brunzelle, J.S.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2020-09-01
Resolution	:	2.05 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 (1)) were used in the production of this report:

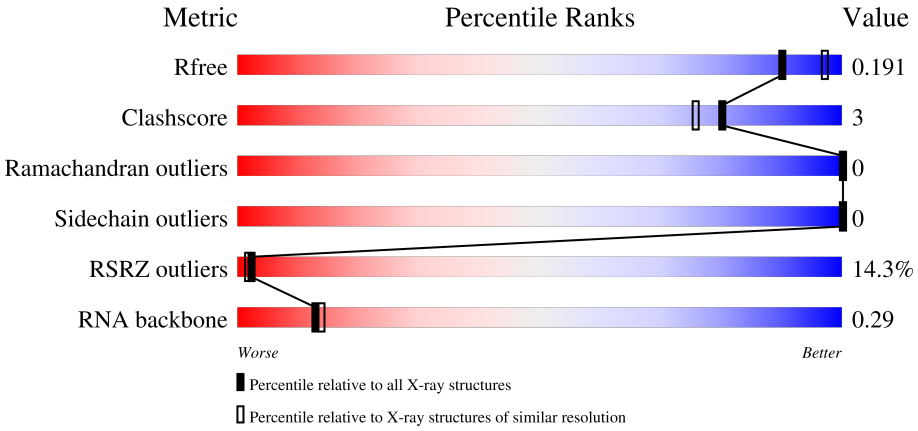
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)
RNA backbone	3102	1018 (2.50-1.58)

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	300	9% 94% 6%
1	C	300	8% 91% 8%
2	B	141	29% 88% 9%
2	D	141	21% 81% 18%

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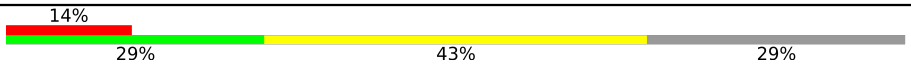
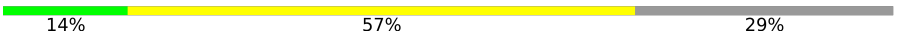
Mol	Chain	Length	Quality of chain
3	E	7	
3	F	7	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7512 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	13	0
			2471	1579	411	464	17			
1	C	297	Total	C	N	O	S	0	10	0
			2408	1540	402	449	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6797	SER	-	expression tag	UNP P0DTD1
A	6798	ASN	-	expression tag	UNP P0DTD1
C	6797	SER	-	expression tag	UNP P0DTD1
C	6798	ASN	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			960	598	161	184	17			
2	D	115	Total	C	N	O	S	0	1	0
			853	531	143	163	16			

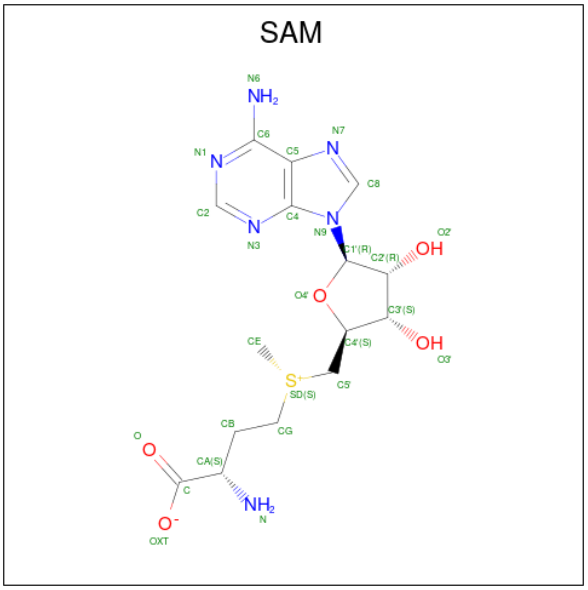
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4252	SER	-	expression tag	UNP P0DTD1
B	4253	ASN	-	expression tag	UNP P0DTD1
D	4252	SER	-	expression tag	UNP P0DTD1
D	4253	ASN	-	expression tag	UNP P0DTD1

- Molecule 3 is a RNA chain called RNA (5'-D(*(M7G))-R(P*AP*UP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	P	0	0	0
			95	39	14	36	6			
3	F	5	Total	C	N	O	P	0	0	0
			95	39	14	36	6			

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

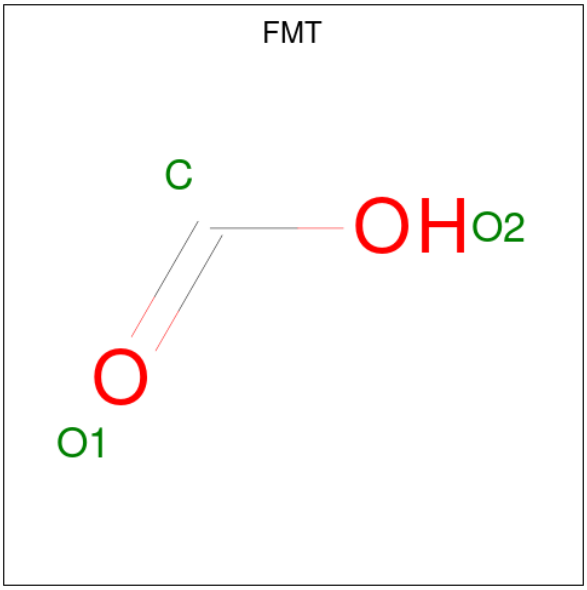
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	C	2	Total Na 2 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 3 1 2	0	0
8	A	1	Total C O 3 1 2	0	0
8	A	1	Total C O 3 1 2	0	0
8	A	1	Total C O 3 1 2	0	0
8	C	1	Total C O 3 1 2	0	0
8	C	1	Total C O 3 1 2	0	0
8	C	1	Total C O 3 1 2	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Zn 2 2	0	0
9	D	2	Total Zn 2 2	0	0

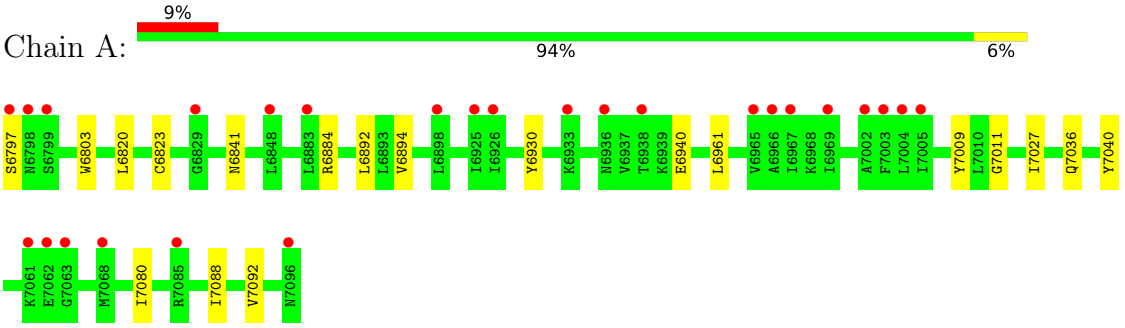
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	209	Total O 222 222	0	18
10	B	38	Total O 38 38	0	1
10	C	212	Total O 224 224	0	14
10	D	44	Total O 44 44	0	0
10	E	7	Total O 7 7	0	0
10	F	10	Total O 10 10	0	0

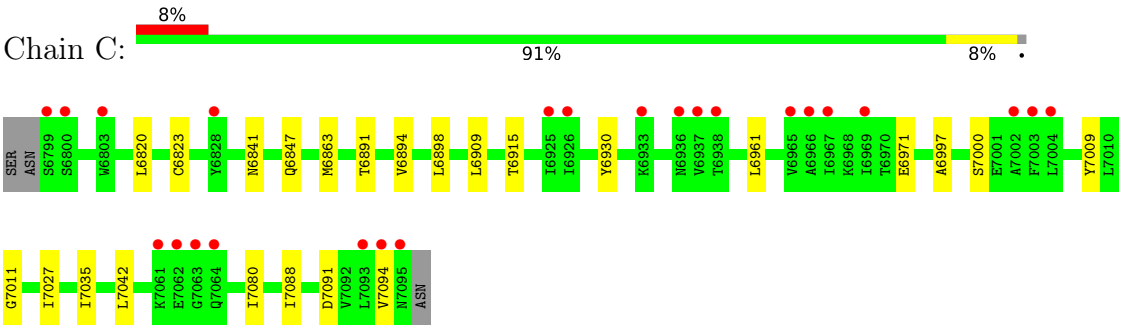
3 Residue-property plots (i)

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.

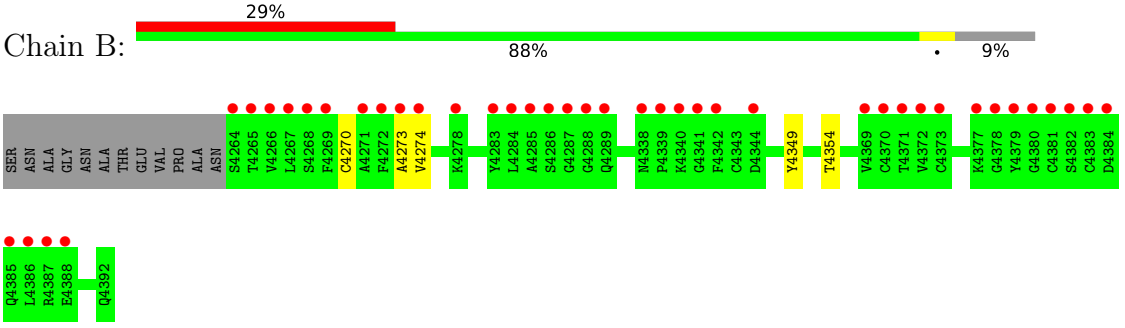
• Molecule 1: 2'-O-methyltransferase



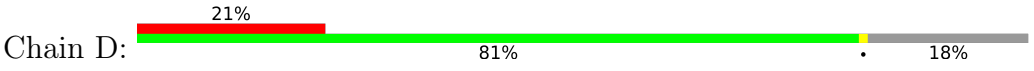
• Molecule 1: 2'-O-methyltransferase

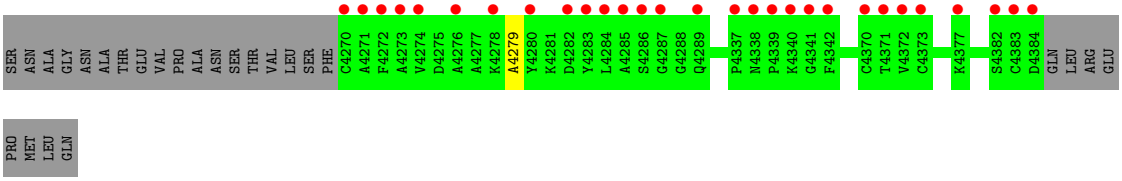


• Molecule 2: Non-structural protein 10

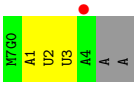


• Molecule 2: Non-structural protein 10

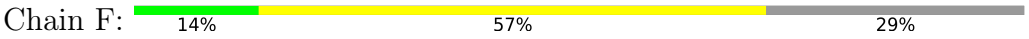


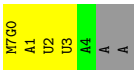


• Molecule 3: RNA (5'-D(*(M7G))-R(P*AP*UP*UP*A)-3')



• Molecule 3: RNA (5'-D(*(M7G))-R(P*AP*UP*UP*A)-3')





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.95Å 166.95Å 98.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 2.05 29.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.97-2.05) 99.9 (29.97-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.166 , 0.185 0.172 , 0.191	Depositor DCC
R_{free} test set	5028 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SAM, NA, M7G, ZN, FMT, MG, CL

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	0.64	0/2526	0.74	0/3429
1	C	0.64	0/2460	0.75	0/3338
2	B	0.71	0/981	0.73	0/1329
2	D	0.71	0/872	0.72	0/1183
3	E	0.30	0/72	0.65	0/110
3	F	0.28	0/72	0.65	0/110
All	All	0.65	0/6983	0.74	0/9499

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	2471	0	2436	16	0
1	C	2408	0	2393	18	0
2	B	960	0	921	5	0
2	D	853	0	812	1	0
3	E	95	0	47	4	0
3	F	95	0	47	5	0
4	A	27	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	27	0	22	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
7	A	1	0	0	0	0
8	A	12	0	4	0	0
8	C	9	0	3	0	0
9	B	2	0	0	0	0
9	D	2	0	0	0	0
10	A	222	0	0	0	0
10	B	38	0	0	1	0
10	C	224	0	0	0	0
10	D	44	0	0	0	0
10	E	7	0	0	0	0
10	F	10	0	0	0	0
All	All	7512	0	6707	37	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 3.

All (37) 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)
2:B:4270:CYS:HA	2:B:4274:VAL:HG12	1.70	0.73
1:A:6940[A]:GLU:N	1:A:6940[A]:GLU:OE1	2.30	0.64
1:C:6820:LEU:HD11	1:C:7027[B]:ILE:HD12	1.81	0.61
1:A:6841:ASN:ND2	3:E:2:U:H4'	2.17	0.60
1:C:6930:TYR:CD1	3:F:1:A:C4	2.93	0.56
1:A:6884:ARG:HB3	2:B:4349:TYR:OH	2.04	0.56
1:C:6971:GLU:OE1	3:F:0:M7G:H82	2.05	0.56
1:C:6820:LEU:CD1	1:C:7027[B]:ILE:HD12	2.36	0.55
2:B:4273:ALA:HB1	2:D:4279:ALA:HB1	1.90	0.54
1:A:6894:VAL:HG11	1:A:7088[A]:ILE:HD12	1.92	0.52
2:B:4274:VAL:O	2:B:4274:VAL:HG13	2.13	0.48
1:A:6797:SER:HB3	1:A:7036:GLN:HB2	1.94	0.48
1:C:6961:LEU:HB2	1:C:7080:ILE:HB	1.96	0.47
1:A:6892:LEU:HD21	1:C:7094:VAL:HG11	1.96	0.46
1:A:6823:CYS:HB2	1:A:7027[A]:ILE:HD12	1.97	0.46
1:C:7009:TYR:CZ	1:C:7011:GLY:HA2	2.50	0.46
1:A:6930:TYR:CD1	3:E:1:A:C4	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7009:TYR:CZ	1:A:7011:GLY:HA2	2.51	0.46
1:C:6915:THR:HB	1:C:7091:ASP:HB2	1.98	0.46
4:A:7101:SAM:CE	3:E:1:A:O2'	2.64	0.45
1:C:6847:GLN:HG3	1:C:7042:LEU:HD21	1.98	0.45
1:A:6841:ASN:HD21	3:E:2:U:H4'	1.82	0.45
1:C:6823:CYS:HB3	3:F:0:M7G:HM73	1.99	0.44
1:C:6841:ASN:ND2	3:F:2:U:H4'	2.33	0.44
1:C:6898[B]:LEU:HG	4:C:7101:SAM:C2	2.48	0.44
1:C:6894:VAL:HG11	1:C:7088[A]:ILE:CD1	2.49	0.43
1:C:6997:ALA:HB1	1:C:7035:ILE:HB	2.01	0.43
2:B:4354:THR:HG21	10:B:4502:HOH:O	2.18	0.42
1:C:6909:LEU:HD11	1:C:7088[A]:ILE:HD12	2.02	0.42
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.00	0.42
1:A:6820:LEU:HD11	1:A:7027[B]:ILE:HD12	2.02	0.41
1:C:6863:MET:HB3	1:C:6891:THR:HG23	2.02	0.41
1:A:7092:VAL:HG22	1:C:7088[A]:ILE:HG13	2.02	0.41
1:A:6803[B]:TRP:HA	1:A:7040[B]:TYR:CD2	2.56	0.41
1:C:7000:SER:HB3	3:F:0:M7G:CM7	2.51	0.41
1:A:6894:VAL:HG11	1:A:7088[A]:ILE:CD1	2.52	0.40
1:A:6820:LEU:CD1	1:A:7027[B]:ILE:HD12	2.52	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	311/300 (104%)	303 (97%)	8 (3%)	0	100	100
1	C	305/300 (102%)	296 (97%)	9 (3%)	0	100	100
2	B	127/141 (90%)	118 (93%)	9 (7%)	0	100	100
2	D	114/141 (81%)	108 (95%)	6 (5%)	0	100	100
All	All	857/882 (97%)	825 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/260 (105%)	273 (100%)	0	100	100
1	C	266/260 (102%)	266 (100%)	0	100	100
2	B	107/115 (93%)	107 (100%)	0	100	100
2	D	94/115 (82%)	94 (100%)	0	100	100
All	All	740/750 (99%)	740 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6972	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	2/7 (28%)	1 (50%)	0
3	F	2/7 (28%)	1 (50%)	0
All	All	4/14 (28%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	3	U
3	F	3	U

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 10 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
8	FMT	C	7107	-	2,2,2	0.26	0	1,1,1	0.16	0
8	FMT	A	7107	-	2,2,2	0.24	0	1,1,1	0.18	0
8	FMT	A	7105	-	2,2,2	0.24	0	1,1,1	0.18	0
4	SAM	C	7101	-	24,29,29	0.71	1 (4%)	23,42,42	1.20	5 (21%)
8	FMT	A	7108	-	2,2,2	0.29	0	1,1,1	0.16	0
8	FMT	C	7105	-	2,2,2	0.27	0	1,1,1	0.21	0
8	FMT	A	7106	-	2,2,2	0.28	0	1,1,1	0.15	0
8	FMT	C	7106	-	2,2,2	0.25	0	1,1,1	0.19	0
4	SAM	A	7101	-	24,29,29	0.75	1 (4%)	23,42,42	1.11	4 (17%)

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
4	SAM	A	7101	-	-	2/12/33/33	0/3/3/3
4	SAM	C	7101	-	-	2/12/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7101	SAM	OXT-C	-2.28	1.23	1.30
4	C	7101	SAM	OXT-C	-2.12	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	7101	SAM	OXT-C-CA	2.79	122.88	113.38
4	C	7101	SAM	C5-C6-N6	2.52	124.19	120.35
4	C	7101	SAM	OXT-C-O	-2.42	118.60	124.09
4	A	7101	SAM	OXT-C-CA	2.40	121.55	113.38
4	A	7101	SAM	C5-C6-N6	2.24	123.75	120.35
4	A	7101	SAM	CG-SD-C5'	-2.08	98.09	103.40
4	C	7101	SAM	O4'-C1'-C2'	-2.08	103.88	106.93
4	C	7101	SAM	CG-SD-C5'	-2.07	98.12	103.40
4	A	7101	SAM	O4'-C1'-C2'	-2.06	103.91	106.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7101	SAM	OXT-C-CA-CB
4	A	7101	SAM	O-C-CA-CB
4	C	7101	SAM	OXT-C-CA-CB
4	C	7101	SAM	O-C-CA-CB

There are no ring outliers.

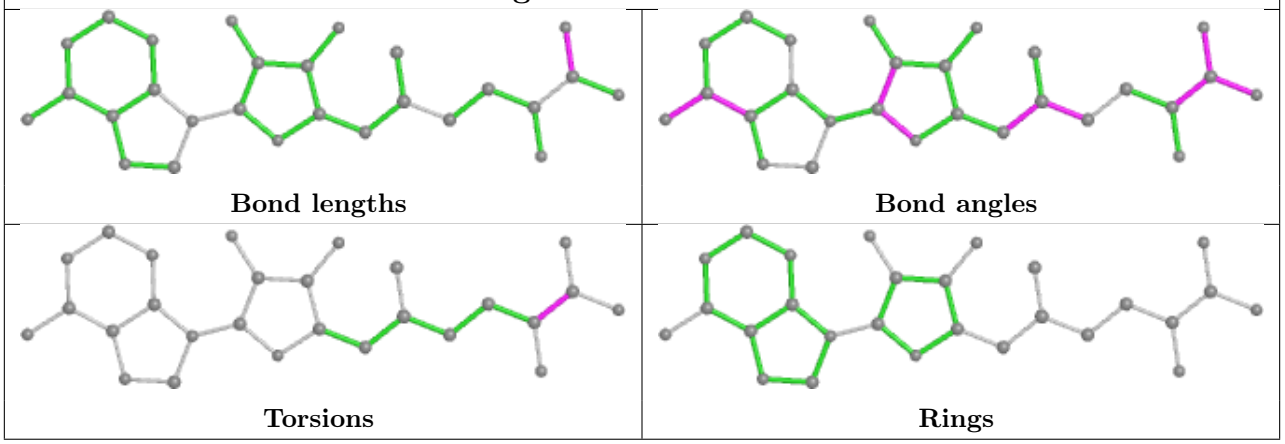
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	7101	SAM	1	0
4	A	7101	SAM	1	0

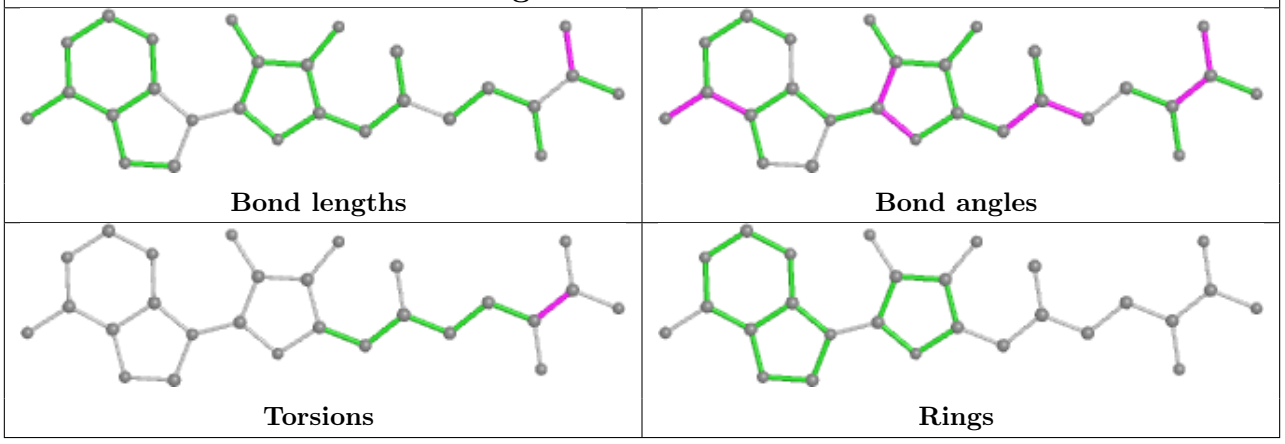
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAM C 7101



Ligand SAM A 7101



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	300/300 (100%)	0.26	26 (8%) 10 10	25, 39, 76, 109	0
1	C	297/300 (99%)	0.18	24 (8%) 12 12	25, 37, 74, 112	0
2	B	129/141 (91%)	1.43	41 (31%) 0 0	36, 70, 117, 132	0
2	D	115/141 (81%)	0.94	29 (25%) 0 0	32, 68, 107, 126	0
3	E	4/7 (57%)	1.12	1 (25%) 0 0	63, 75, 120, 132	0
3	F	4/7 (57%)	0.11	0 100 100	63, 70, 89, 120	0
All	All	849/896 (94%)	0.51	121 (14%) 2 2	25, 43, 98, 132	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	4383	CYS	9.1
2	B	4339	PRO	8.8
2	B	4386	LEU	8.3
2	D	4270	CYS	7.9
2	B	4273	ALA	7.8
2	B	4272	PHE	7.6
1	C	6938	THR	7.0
2	D	4382	SER	6.8
2	B	4267	LEU	6.6
2	B	4271	ALA	6.2
2	B	4383	CYS	6.1
2	B	4340	LYS	5.9
1	A	6797	SER	5.7
2	B	4342	PHE	5.6
2	D	4339	PRO	5.6
2	B	4384	ASP	5.6
2	B	4387	ARG	5.5
2	D	4271	ALA	5.4
2	B	4274	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	4265	THR	5.3
2	D	4384	ASP	5.2
1	C	7062	GLU	5.1
2	D	4372	VAL	5.1
2	B	4372	VAL	5.0
2	B	4285	ALA	5.0
2	B	4382	SER	5.0
2	B	4286	SER	4.9
1	C	7093	LEU	4.8
2	B	4385	GLN	4.7
1	C	7061	LYS	4.6
2	B	4287	GLY	4.5
1	C	6799	SER	4.5
2	D	4284	LEU	4.5
2	D	4285	ALA	4.4
2	D	4340	LYS	4.3
2	B	4373	CYS	4.3
1	A	6799	SER	4.1
1	A	7096	ASN	4.1
1	A	7061	LYS	4.0
1	A	7062	GLU	4.0
1	A	6829	GLY	3.9
2	B	4381	CYS	3.8
2	B	4288	GLY	3.7
2	D	4341	GLY	3.7
1	A	7085	ARG	3.7
2	D	4287	GLY	3.6
2	D	4371	THR	3.5
1	A	6938	THR	3.4
2	D	4278	LYS	3.4
1	C	7063	GLY	3.4
1	C	6967	ILE	3.4
2	B	4371	THR	3.3
2	B	4264	SER	3.3
2	B	4341	GLY	3.3
1	C	6933	LYS	3.3
2	B	4268	SER	3.2
2	D	4342	PHE	3.2
1	C	7004	LEU	3.2
2	B	4284	LEU	3.2
1	C	6937	VAL	3.2
1	C	6966	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	6798	ASN	3.1
1	C	7003	PHE	3.1
1	A	7068	MET	3.1
1	A	6926	ILE	3.1
2	B	4289	GLN	3.1
2	B	4377	LYS	3.1
2	D	4286	SER	3.0
2	D	4289	GLN	3.0
1	A	6925	ILE	3.0
2	B	4283	TYR	3.0
1	C	7095	ASN	3.0
1	A	7003	PHE	2.9
2	D	4283	TYR	2.9
1	A	7004	LEU	2.9
1	C	6926	ILE	2.9
2	B	4369	VAL	2.9
2	D	4337	PRO	2.9
2	B	4380	GLY	2.9
1	A	6967	ILE	2.8
1	A	6966	ALA	2.8
2	D	4338	ASN	2.8
1	C	7094	VAL	2.8
1	C	6800	SER	2.8
2	B	4266	VAL	2.8
1	A	7002	ALA	2.8
1	C	6965	VAL	2.8
1	C	6969	ILE	2.8
1	A	7063	GLY	2.8
1	C	6936	ASN	2.7
2	B	4370	CYS	2.7
1	A	6936	ASN	2.7
2	B	4338	ASN	2.7
1	A	6848	LEU	2.7
2	B	4278	LYS	2.7
2	B	4269	PHE	2.7
2	D	4273	ALA	2.7
1	A	6933	LYS	2.7
1	C	6925	ILE	2.7
2	D	4377	LYS	2.6
2	D	4282	ASP	2.6
2	D	4373	CYS	2.5
2	D	4272	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	4388	GLU	2.4
1	C	7064	GLN	2.4
2	D	4274	VAL	2.4
1	A	7005	ILE	2.4
1	A	6969	ILE	2.3
1	C	7002	ALA	2.2
2	B	4378	GLY	2.2
2	B	4344	ASP	2.2
2	D	4370	CYS	2.2
2	D	4280	TYR	2.2
1	A	6898[A]	LEU	2.2
1	C	6828	TYR	2.1
2	D	4276	ALA	2.1
1	C	6803	TRP	2.1
3	E	4	A	2.1
2	B	4379	TYR	2.1
1	A	6965	VAL	2.0
1	A	6883	LEU	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 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
6	NA	A	7103	1/1	0.83	0.08	64,64,64,64	0
9	ZN	D	4402	1/1	0.86	0.10	66,66,66,66	1
8	FMT	A	7108	3/3	0.88	0.17	67,67,72,72	0
9	ZN	B	4402	1/1	0.90	0.11	61,61,61,61	1
8	FMT	C	7107	3/3	0.90	0.14	53,53,54,56	0

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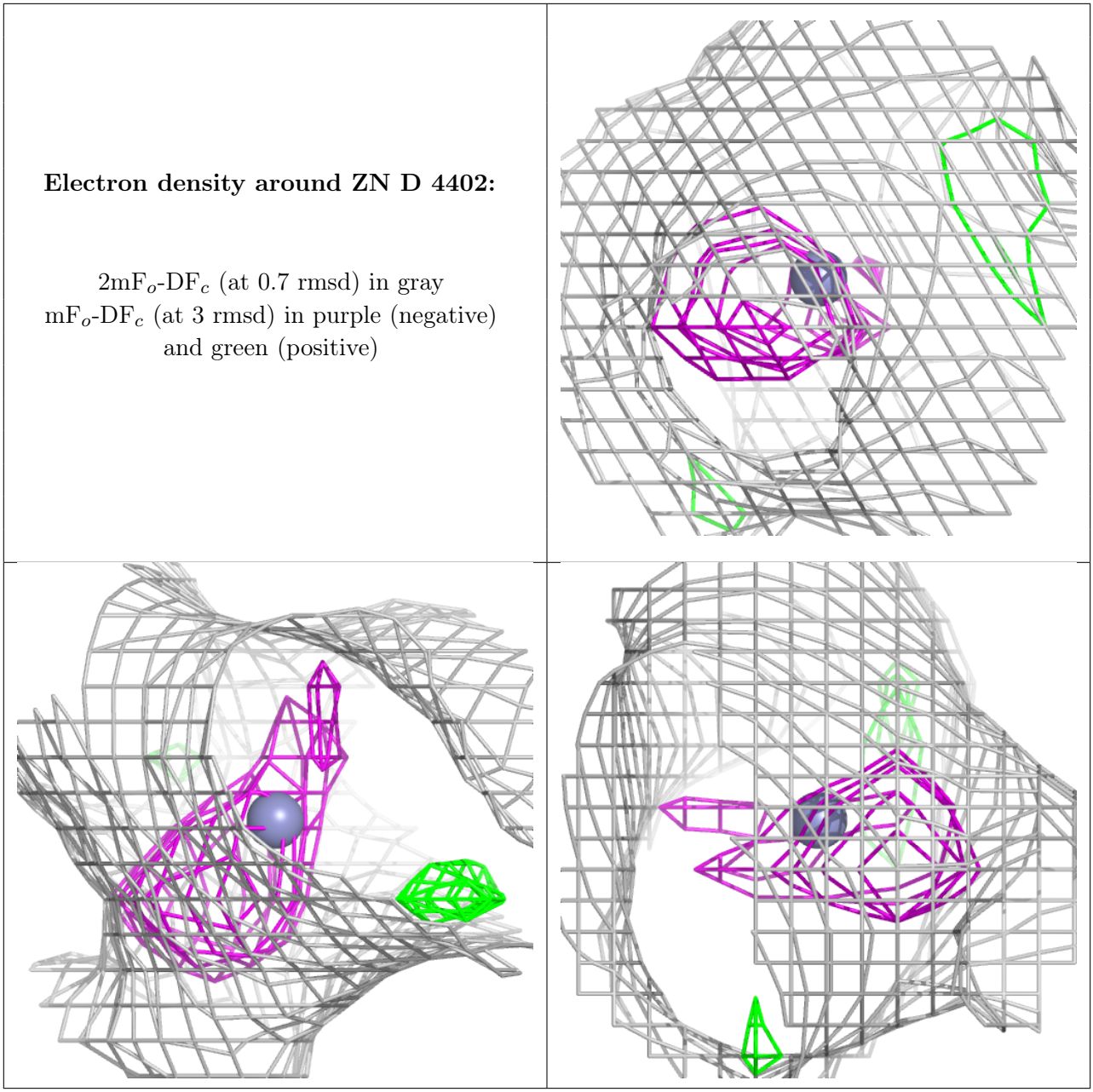
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	7102	1/1	0.91	0.17	42,42,42,42	1
6	NA	C	7104	1/1	0.94	0.15	50,50,50,50	0
4	SAM	C	7101	27/27	0.95	0.08	33,36,38,43	0
8	FMT	A	7107	3/3	0.95	0.14	58,58,59,62	0
6	NA	C	7103	1/1	0.95	0.51	64,64,64,64	0
8	FMT	A	7106	3/3	0.96	0.09	62,62,65,67	0
5	MG	C	7102	1/1	0.96	0.23	42,42,42,42	1
8	FMT	C	7106	3/3	0.97	0.13	51,51,56,58	0
4	SAM	A	7101	27/27	0.97	0.07	34,35,36,39	0
7	CL	A	7104	1/1	0.98	0.12	86,86,86,86	0
9	ZN	B	4401	1/1	0.98	0.04	55,55,55,55	0
8	FMT	C	7105	3/3	0.98	0.06	38,38,39,39	0
9	ZN	D	4401	1/1	0.98	0.04	49,49,49,49	0
8	FMT	A	7105	3/3	0.98	0.13	56,56,59,60	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.

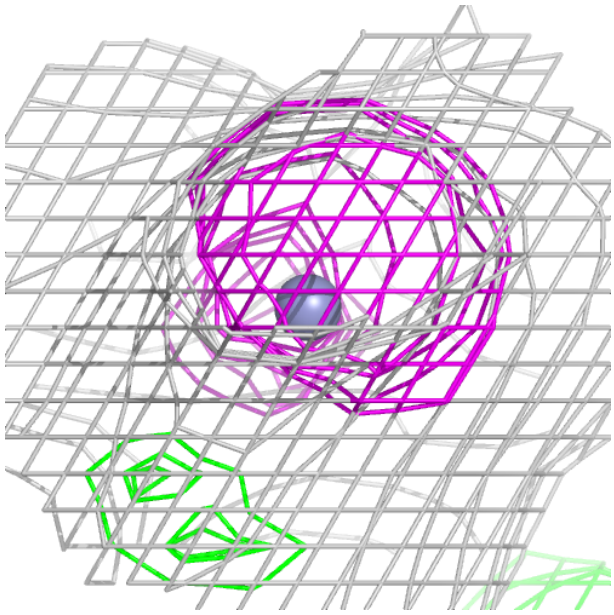
Electron density around ZN D 4402:

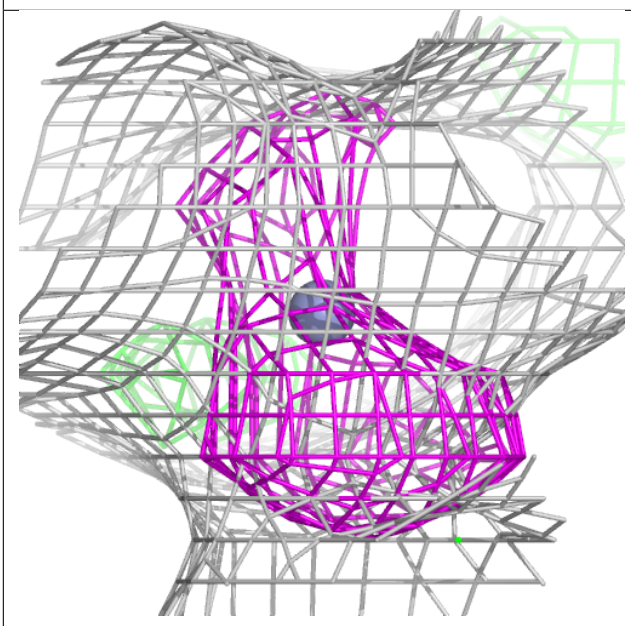
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

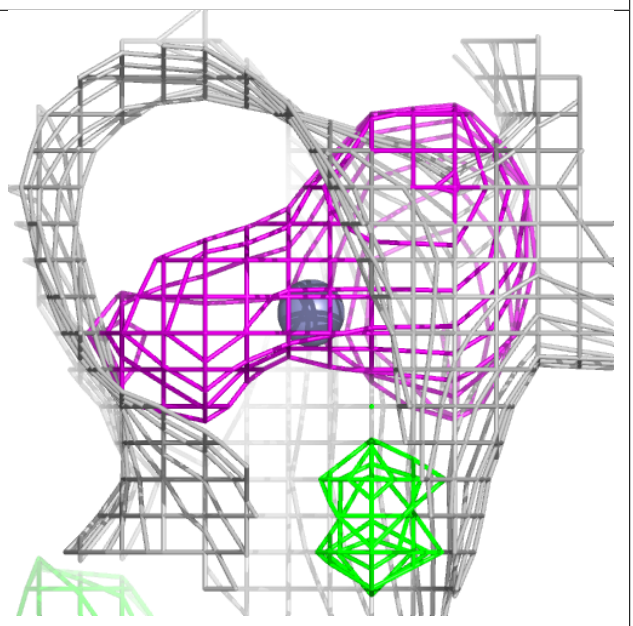


Electron density around ZN B 4402:

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

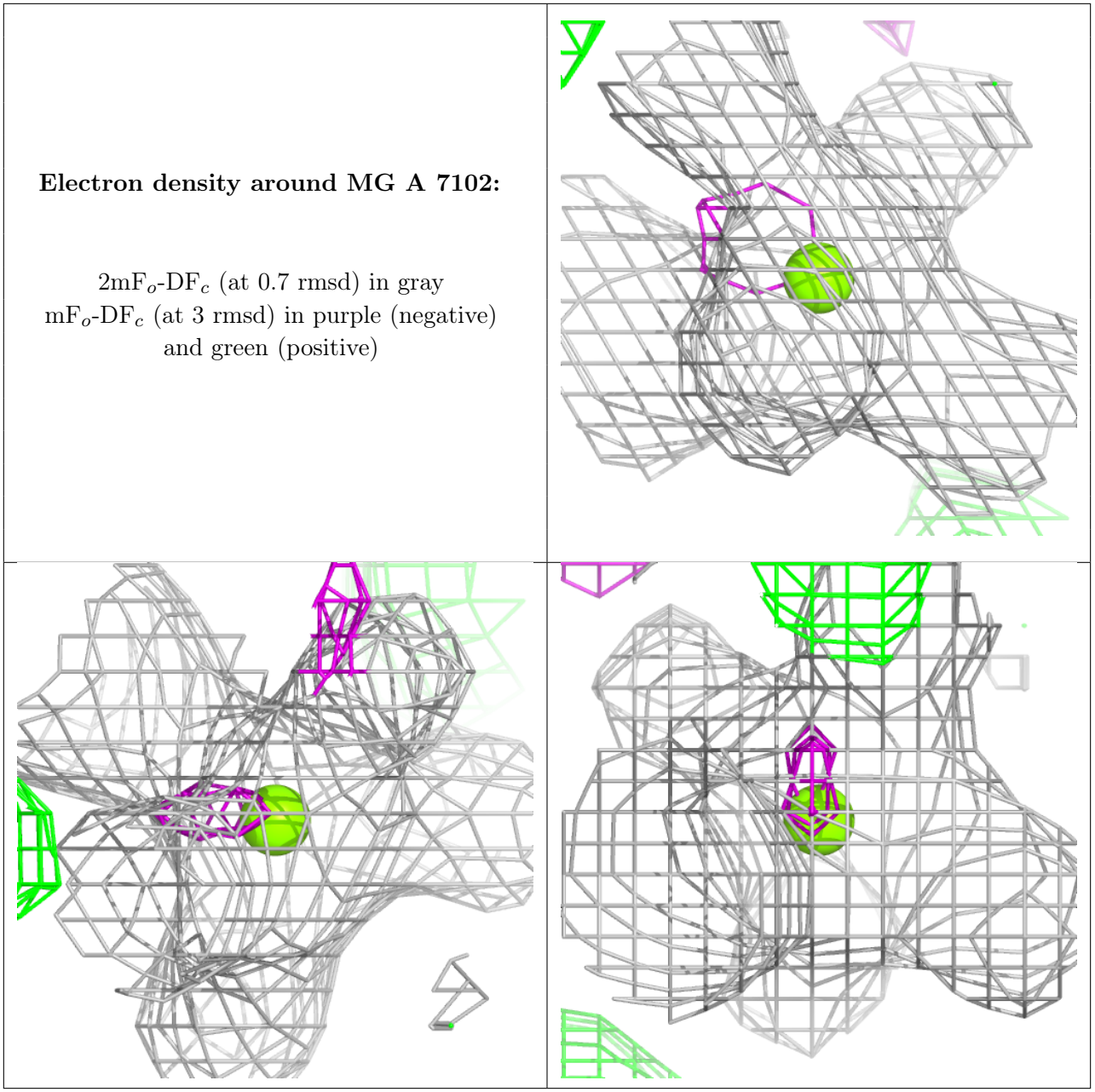






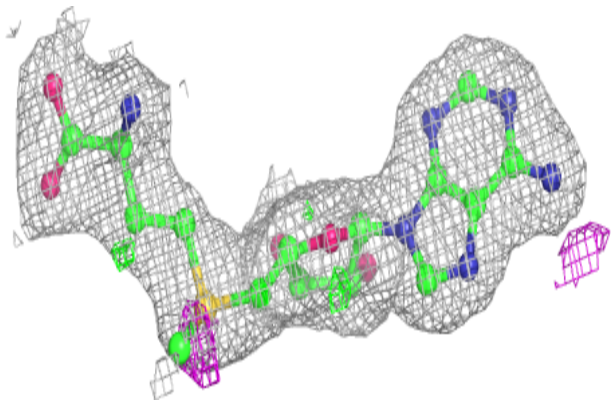
Electron density around MG A 7102:

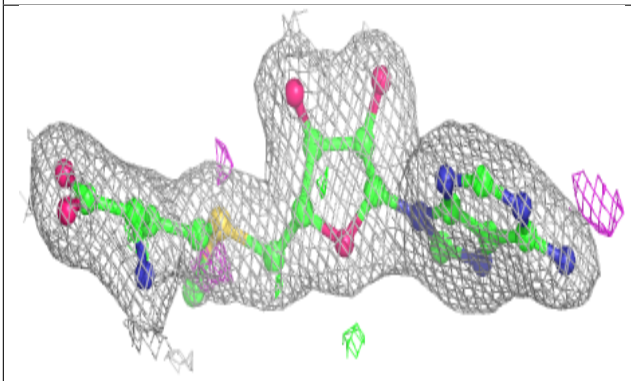
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

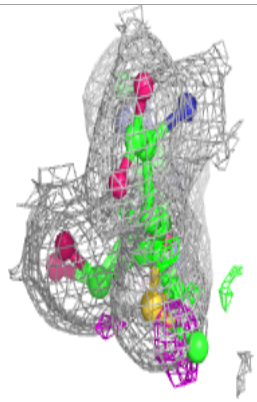


Electron density around SAM C 7101:

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

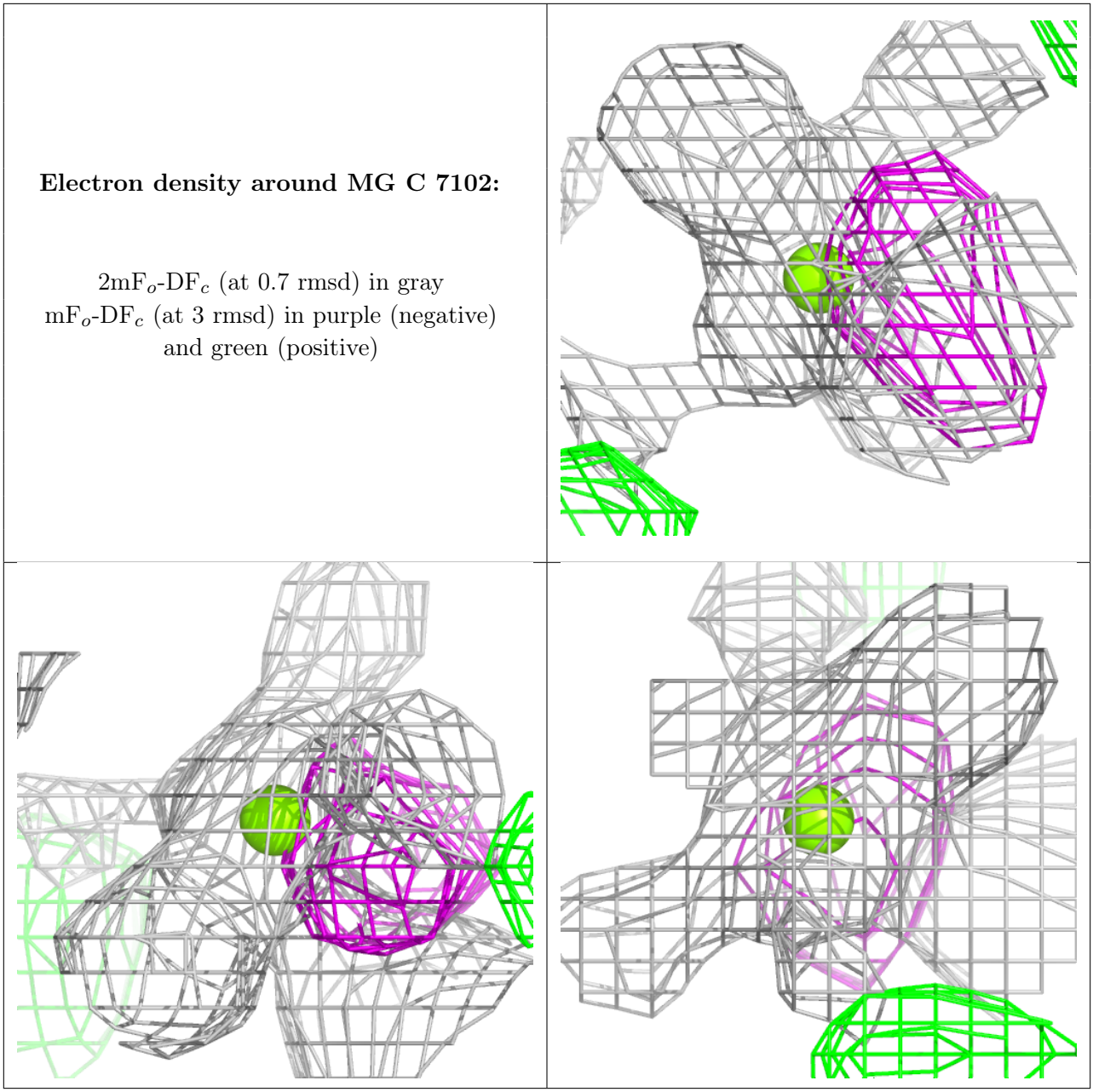






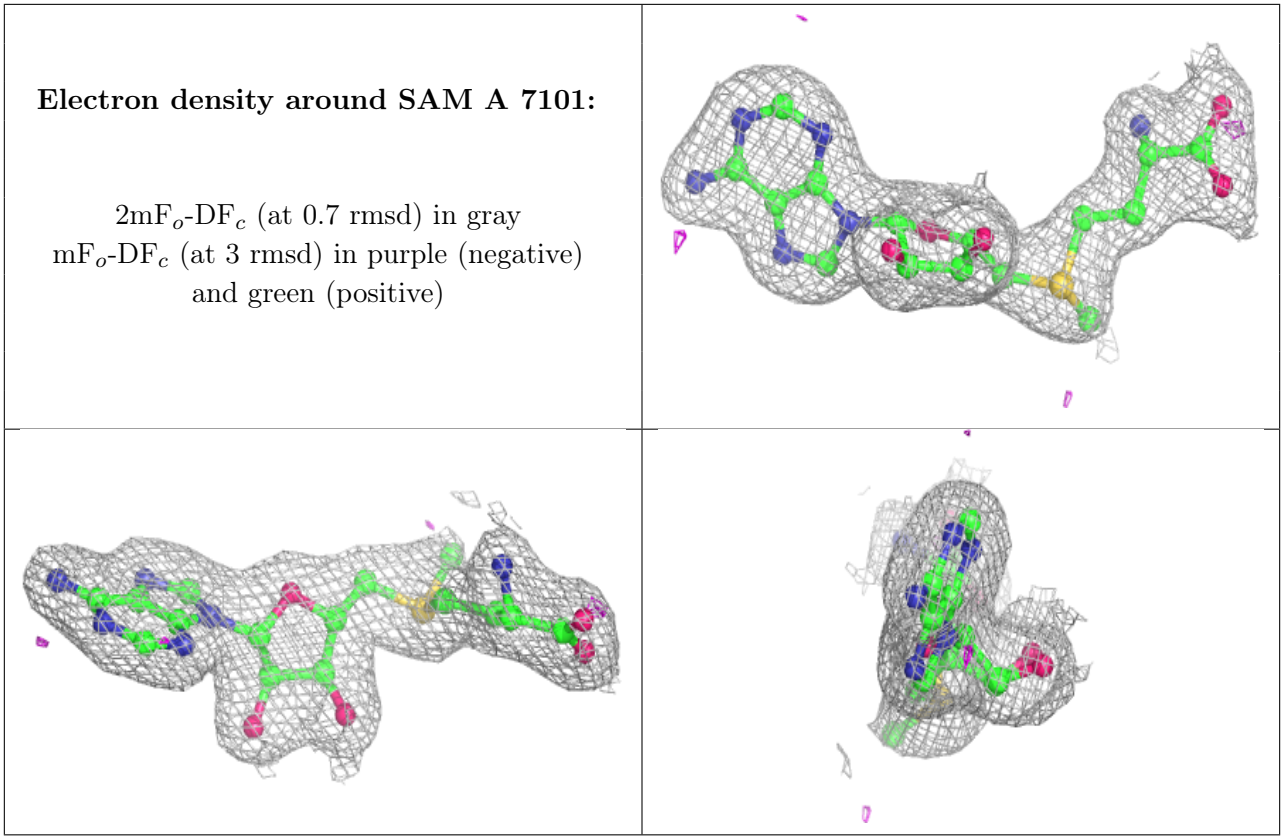
Electron density around MG C 7102:

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



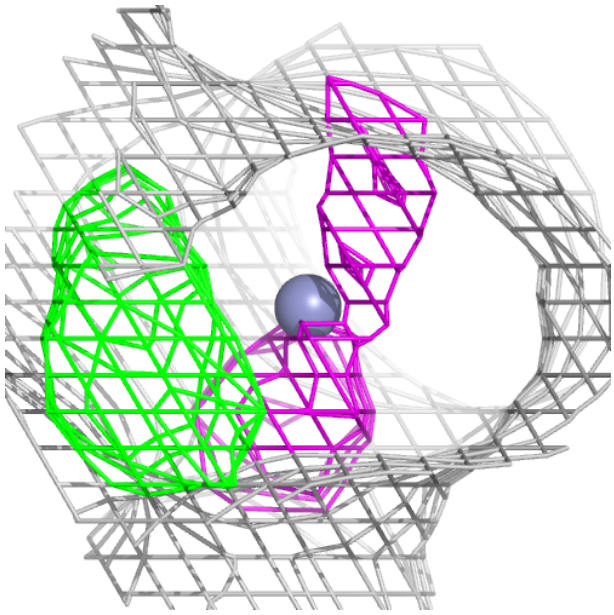
Electron density around SAM A 7101:

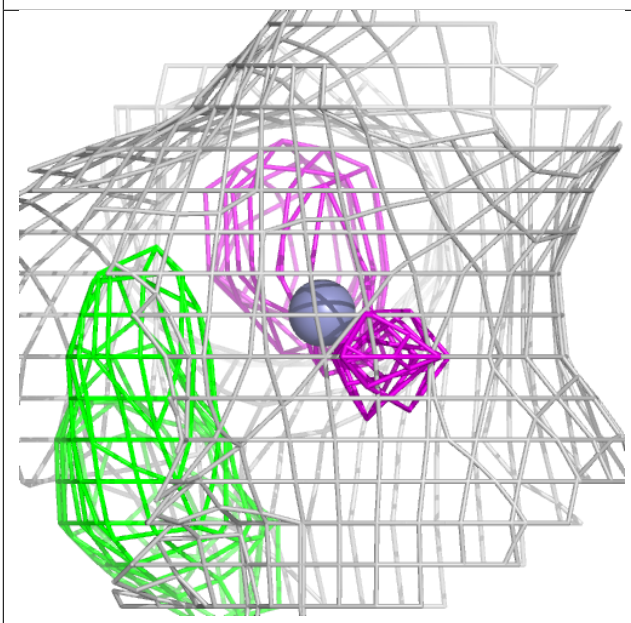
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

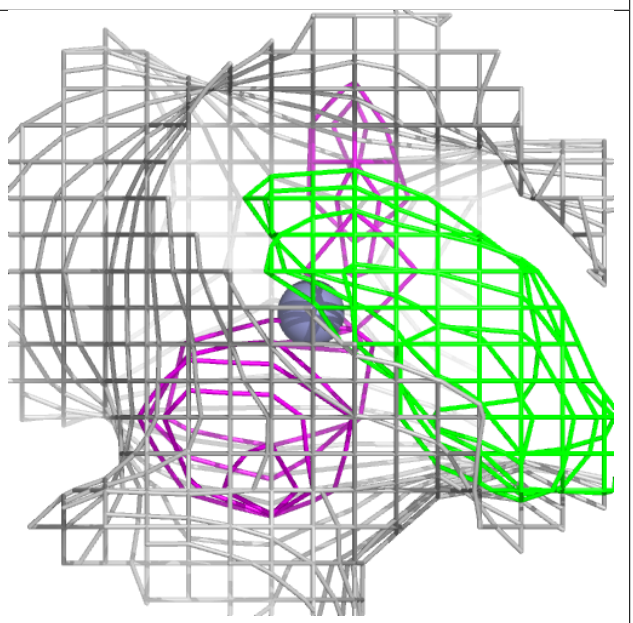


Electron density around ZN B 4401:

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

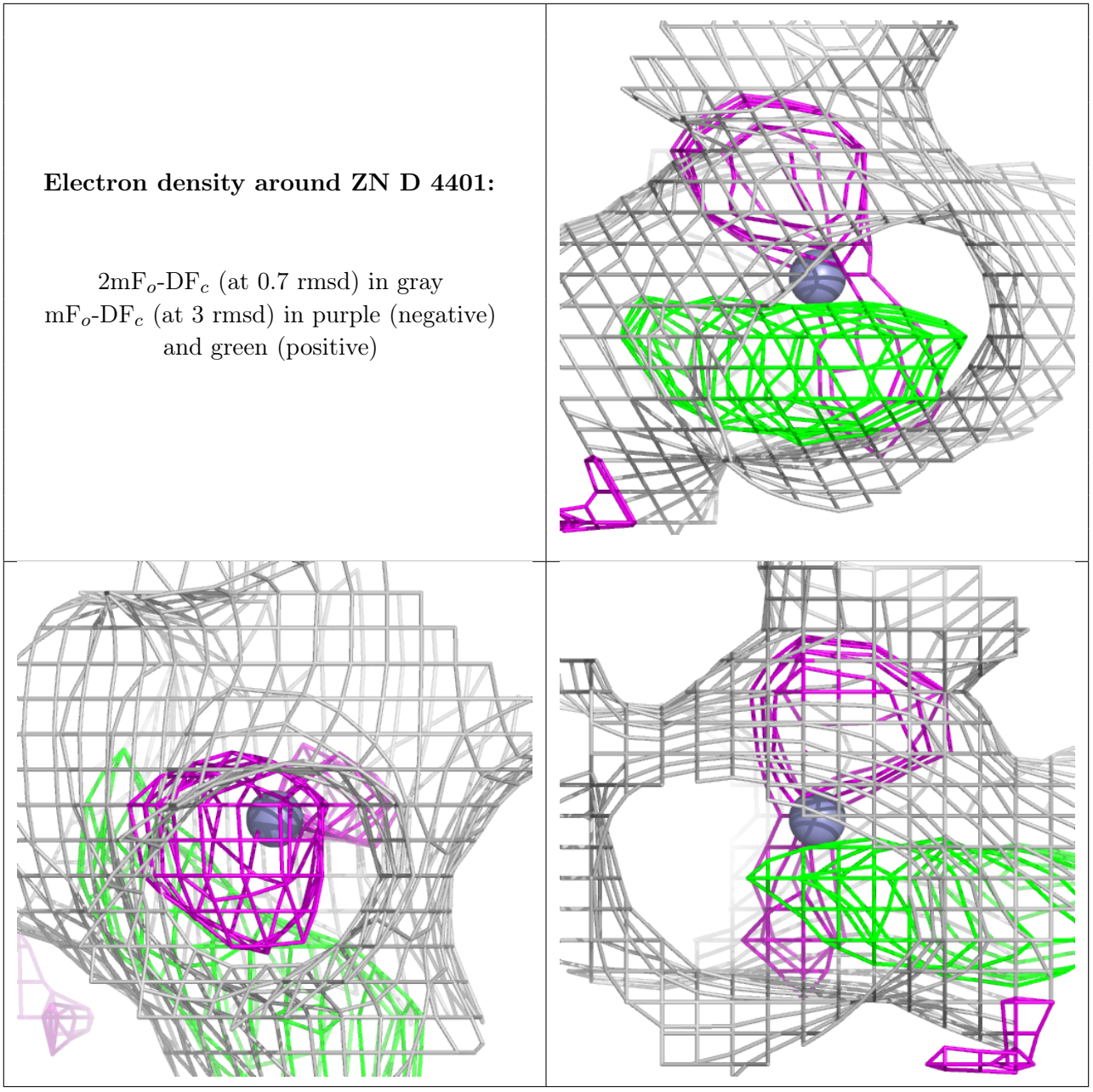






Electron density around ZN D 4401:

$2mF_o$-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 (i)

There are no such residues in this entry.