



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 10:23 am BST

PDB ID : 8BO1
Title : ExoY Nucleotidyl Cyclase domain from *Vibrio nigrripulchritudo* MARTX toxin, bound to Latrunculin-B-ATP-Mg-actin, and 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE and 2 Mg ions
Authors : Teixeira-Nunes, M.; Renault, L.; Retailleau, P.
Deposited on : 2022-11-14
Resolution : 2.50 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

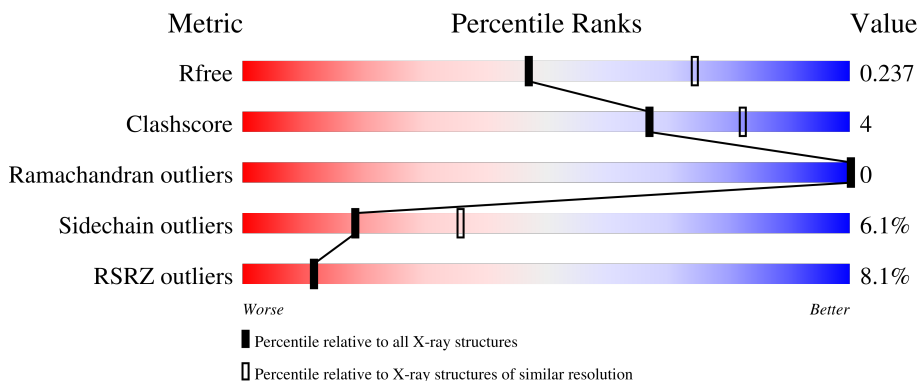
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

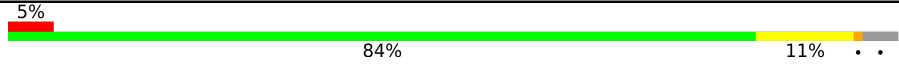



The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	375	 5% 84% 11% . .
1	C	375	 13% 85% 12% . .
2	B	413	 8% 83% 11% . .
2	D	413	 7% 81% 12% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	404	-	-	-	X
6	SO4	C	405	-	-	-	X

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 12368 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 Actin, alpha skeletal muscle, intermediate form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2804	1778	469	539	18	0	0	0
1	C	364	2845	1803	479	544	19	0	1	0

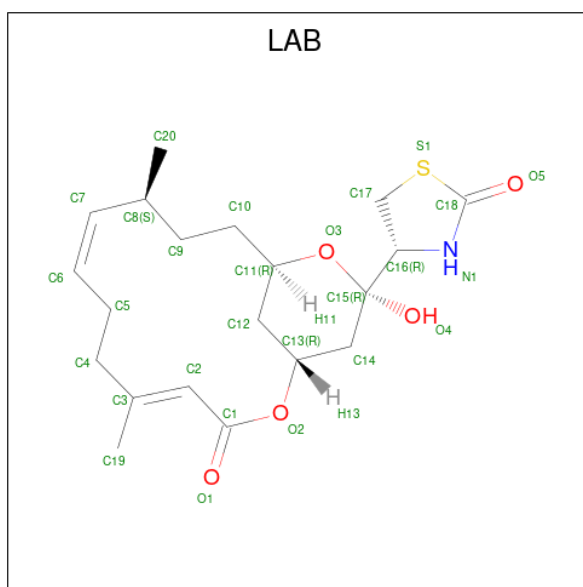
- Molecule 2 is a protein called Putative Adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	398	3144	1992	519	624	9	0	0	0
2	D	396	3134	1984	519	622	9	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

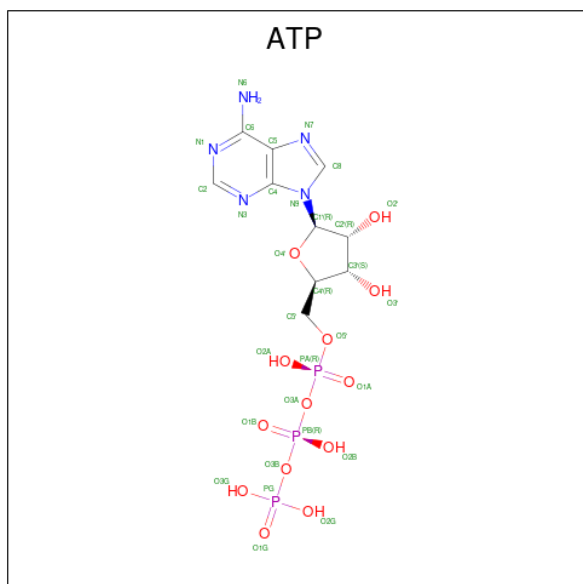
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	GLY	-	expression tag	UNP A0A6N3LUE9
B	452	PRO	-	expression tag	UNP A0A6N3LUE9
B	453	GLY	-	expression tag	UNP A0A6N3LUE9
B	454	SER	-	expression tag	UNP A0A6N3LUE9
D	451	GLY	-	expression tag	UNP A0A6N3LUE9
D	452	PRO	-	expression tag	UNP A0A6N3LUE9
D	453	GLY	-	expression tag	UNP A0A6N3LUE9
D	454	SER	-	expression tag	UNP A0A6N3LUE9

- Molecule 3 is LATRUNCULIN B (three-letter code: LAB) (formula: C₂₀H₂₉NO₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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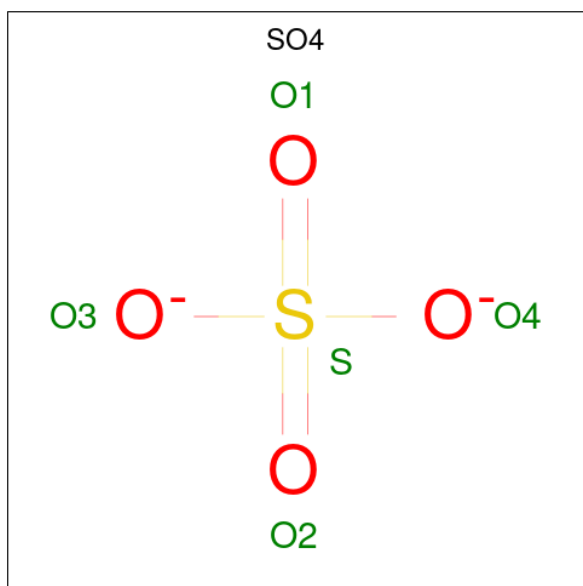
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	31	10	5	13	3	0	0

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

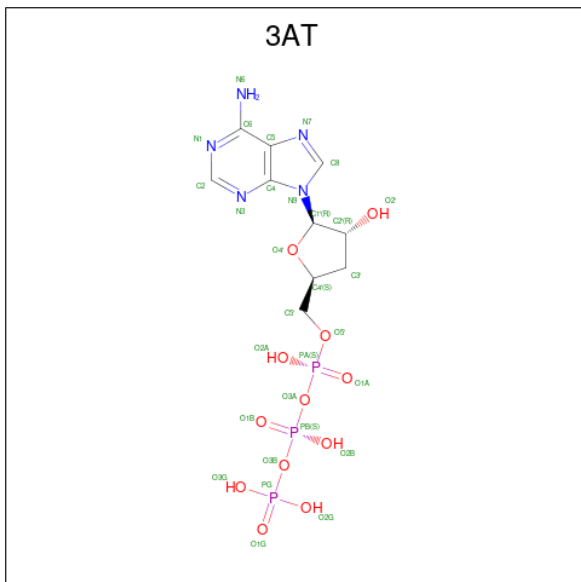
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	B	2	2	2	0	2
5	C	1	1	1	0	1
5	D	2	2	2	0	2

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

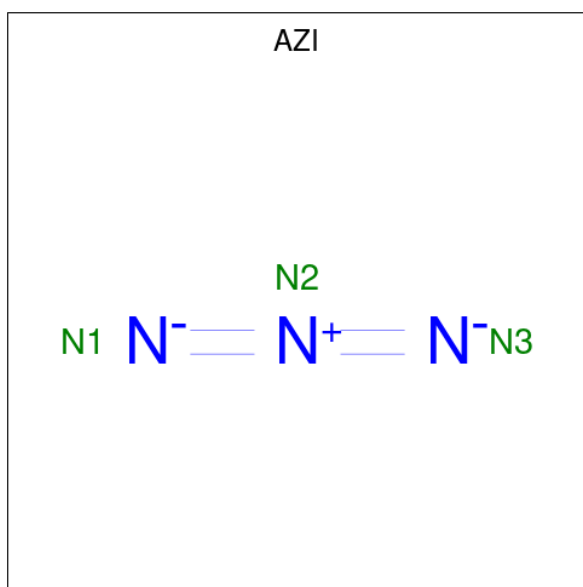


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	30	10	5	12	3	0	0
7	D	1	30	10	5	12	3	0	0

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
8	B	2	2	2	0	2
8	C	1	1	1	0	1
8	D	5	5	5	0	2

- Molecule 9 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total N 3 3	0	0
9	D	1	Total N 3 3	0	0
9	D	1	Total N 3 3	0	0
9	D	1	Total N 3 3	0	0
9	D	1	Total N 3 3	0	0
9	D	1	Total N 3 3	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Cl 2 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	55	Total O 55 55	0	0
11	B	55	Total O 55 55	0	0

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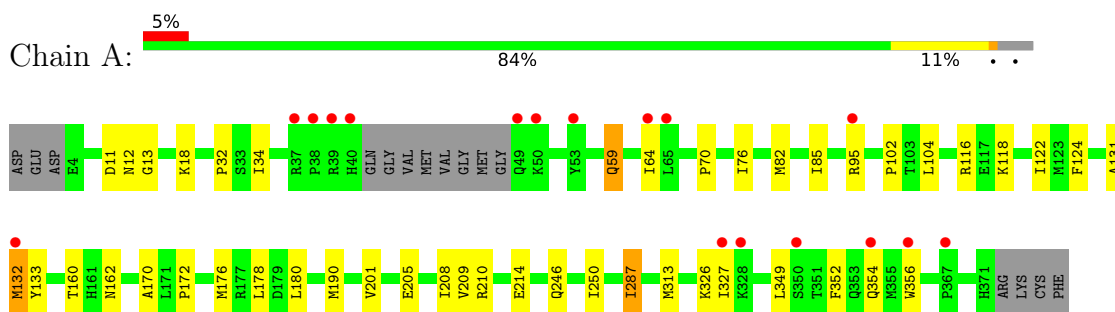
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	21	Total	O	0	0
			21	21		
11	D	85	Total	O	0	0
			85	85		

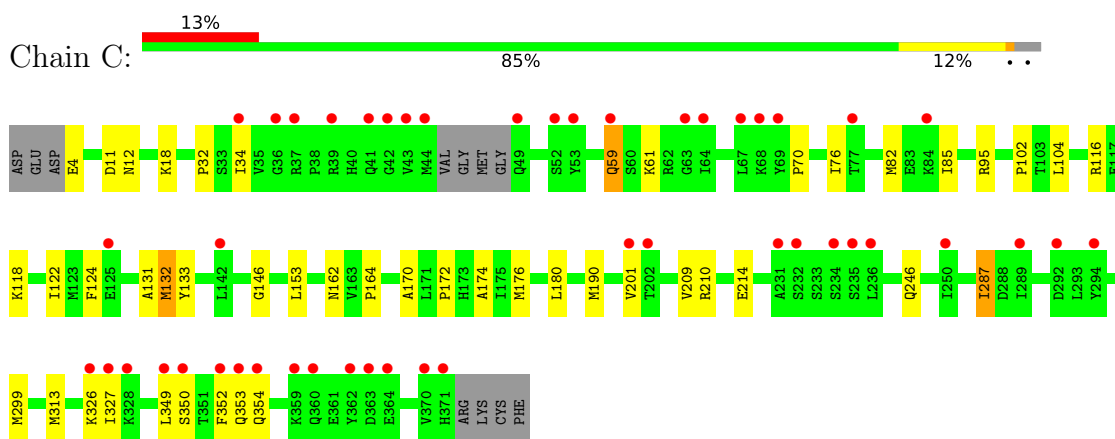
3 Residue-property plots [i](#)

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.

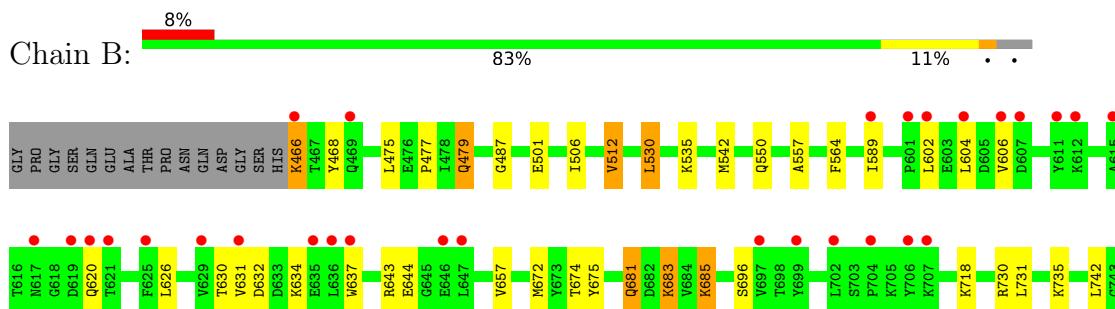
- Molecule 1: Actin, alpha skeletal muscle, intermediate form



- Molecule 1: Actin, alpha skeletal muscle, intermediate form

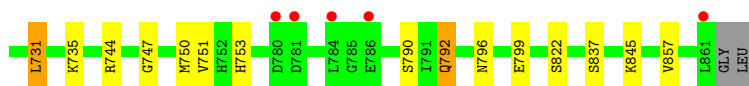
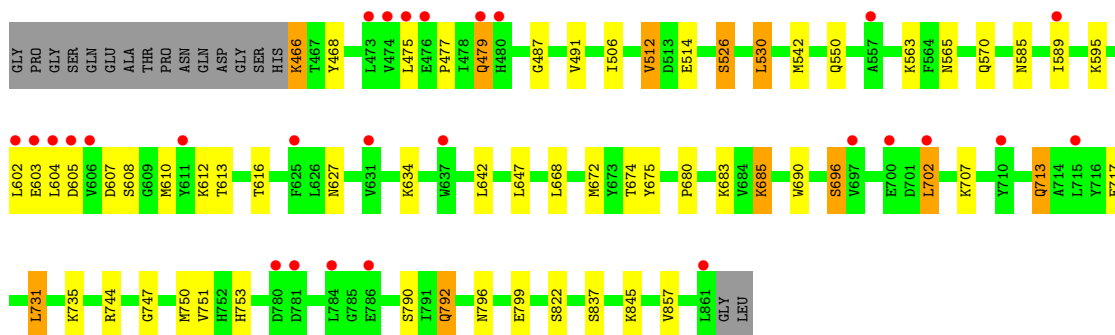
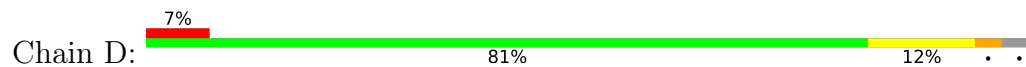


- Molecule 2: Putative Adenylate cyclase





● Molecule 2: Putative Adenylate cyclase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.50Å 132.17Å 96.03Å 90.00° 110.80° 90.00°	Depositor
Resolution (Å)	48.24 – 2.50 48.24 – 2.50	Depositor EDS
% Data completeness (in resolution range)	74.1 (48.24-2.50) 74.1 (48.24-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.51Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.191 , 0.231 0.192 , 0.237	Depositor DCC
R_{free} test set	2243 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LAB, AZI, CL, MN, SO4, 3AT, MG, ATP

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	0.41	0/2864	0.57	0/3884
1	C	0.38	0/2909	0.56	0/3943
2	B	0.44	0/3212	0.62	0/4353
2	D	0.46	0/3202	0.63	0/4340
All	All	0.43	0/12187	0.60	0/16520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2804	0	2762	21	0
1	C	2845	0	2809	23	0
2	B	3144	0	3056	22	0
2	D	3134	0	3042	30	0
3	A	27	0	29	1	0
3	C	27	0	29	1	0
4	A	31	0	12	0	0
4	C	31	0	12	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	30	0	12	0	0
7	D	30	0	12	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
8	D	5	0	0	0	0
9	D	18	0	0	0	0
10	D	2	0	0	0	0
11	A	55	0	0	1	0
11	B	55	0	0	0	0
11	C	21	0	0	0	0
11	D	85	0	0	2	0
All	All	12368	0	11775	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (94) 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:631:VAL:HG13	2:B:632:ASP:H	1.48	0.78
1:C:59:GLN:HB2	3:C:401:LAB:H7	1.72	0.71
1:A:59:GLN:HB2	3:A:401:LAB:H7	1.73	0.68
2:D:744:ARG:CD	2:D:750:MET:HG2	2.25	0.67
1:C:287:ILE:H	1:C:287:ILE:HD12	1.64	0.62
2:D:744:ARG:HD3	2:D:750:MET:HG2	1.80	0.62
2:D:610:MET:HE2	2:D:627:ASN:HB2	1.82	0.62
1:A:287:ILE:HD12	1:A:287:ILE:H	1.65	0.60
2:B:631:VAL:HG13	2:B:632:ASP:N	2.15	0.60
2:B:799:GLU:CD	2:B:799:GLU:H	2.07	0.58
1:C:326:LYS:NZ	1:C:327:ILE:H	2.04	0.56
2:D:799:GLU:H	2:D:799:GLU:CD	2.09	0.56
2:D:790:SER:HB2	2:D:792:GLN:OE1	2.06	0.56
2:B:790:SER:HB2	2:B:792:GLN:OE1	2.06	0.56
2:B:683:LYS:HG2	2:B:685:LYS:HD2	1.87	0.56
1:A:104:LEU:HD13	1:A:133:TYR:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:HD13	1:C:133:TYR:HD2	1.71	0.55
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.89	0.55
2:D:702:LEU:HB3	2:D:707:LYS:HG3	1.87	0.55
1:A:326:LYS:NZ	1:A:327:ILE:H	2.04	0.55
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.89	0.55
1:C:61:LYS:HE3	2:D:696:SER:HA	1.88	0.54
2:D:683:LYS:HG2	2:D:685:LYS:HD2	1.88	0.54
2:B:832:ASN:HA	2:B:835:LEU:HD22	1.90	0.54
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.91	0.53
1:A:76:ILE:HD13	1:A:82:MET:HG2	1.91	0.53
1:C:76:ILE:HD13	1:C:82:MET:HG2	1.91	0.53
2:D:713:GLN:NE2	2:D:717:GLU:OE2	2.43	0.52
1:C:350:SER:HA	1:C:353:GLN:HG2	1.91	0.52
2:D:585:ASN:O	2:D:589:ILE:HG12	2.10	0.51
2:B:735:LYS:HG3	2:B:751:VAL:HG12	1.92	0.51
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.94	0.50
1:C:326:LYS:HZ1	1:C:327:ILE:H	1.58	0.50
2:B:631:VAL:CG1	2:B:632:ASP:H	2.23	0.50
2:D:735:LYS:HG3	2:D:751:VAL:HG12	1.93	0.50
1:C:190:MET:HG3	1:C:209:VAL:HG11	1.94	0.49
1:C:170:ALA:O	1:C:172:PRO:HD3	2.11	0.49
2:D:487:GLY:HA2	2:D:514:GLU:HA	1.94	0.49
2:B:550:GLN:HG2	2:B:564:PHE:HB3	1.93	0.49
2:D:603:GLU:HB3	2:D:612:LYS:HB3	1.94	0.49
1:A:190:MET:HG3	1:A:209:VAL:HG11	1.94	0.48
2:D:602:LEU:HD23	2:D:613:THR:HB	1.95	0.48
2:B:589:ILE:HG13	2:B:637:TRP:CD1	2.48	0.48
2:D:605:ASP:HA	2:D:610:MET:O	2.12	0.48
2:D:512:VAL:HG13	11:D:1330:HOH:O	2.13	0.48
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.95	0.47
2:D:526:SER:HB3	2:D:747:GLY:O	2.14	0.47
1:A:170:ALA:O	1:A:172:PRO:HD3	2.15	0.47
2:D:690:TRP:CD2	2:D:713:GLN:HB2	2.50	0.47
2:B:535:LYS:HB2	2:B:557:ALA:HB2	1.96	0.47
2:D:530:LEU:HD13	2:D:753:HIS:CG	2.50	0.47
2:B:487:GLY:HA3	2:B:512:VAL:HG22	1.96	0.47
1:C:118:LYS:HE3	1:C:122:ILE:HD11	1.96	0.47
1:C:146:GLY:HA2	2:D:857:VAL:HG23	1.96	0.47
2:B:466:LYS:O	2:B:477:PRO:HG3	2.15	0.47
1:A:118:LYS:HE3	1:A:122:ILE:HD11	1.98	0.46
1:A:13:GLY:HA2	11:A:523:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:LEU:O	1:C:352:PHE:HB3	2.16	0.46
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.98	0.45
1:A:352:PHE:CE2	1:A:356:TRP:NE1	2.85	0.45
2:D:680:PRO:HD2	11:D:1347:HOH:O	2.16	0.45
2:B:479:GLN:H	2:B:479:GLN:CD	2.20	0.45
2:D:530:LEU:HD13	2:D:753:HIS:CB	2.47	0.45
1:C:153:LEU:HD23	1:C:299:MET:HE2	1.99	0.44
2:D:466:LYS:O	2:D:477:PRO:HG3	2.17	0.44
2:D:550:GLN:HB2	2:D:565:ASN:OD1	2.18	0.44
1:A:32:PRO:HB2	1:A:34:ILE:HG12	2.00	0.43
2:B:742:LEU:HB3	2:B:744:ARG:HG2	2.00	0.43
2:B:530:LEU:HD13	2:B:753:HIS:CG	2.53	0.43
1:C:70:PRO:HG2	1:C:85:ILE:HD12	2.00	0.43
1:C:210:ARG:O	1:C:214:GLU:HG3	2.18	0.43
2:B:631:VAL:HG12	2:B:634:LYS:HB2	2.00	0.43
2:B:681:GLN:HG3	2:B:730:ARG:HB2	1.99	0.43
1:A:210:ARG:O	1:A:214:GLU:HG3	2.19	0.43
2:B:506:ILE:HB	2:B:672:MET:HB2	2.01	0.43
1:C:11:ASP:HB3	1:C:18:LYS:HB2	2.01	0.42
2:D:607:ASP:O	2:D:608:SER:HB3	2.19	0.42
2:D:668:LEU:HD12	2:D:731:LEU:HD21	2.00	0.42
1:A:11:ASP:HB3	1:A:18:LYS:HB2	2.01	0.42
1:A:349:LEU:O	1:A:352:PHE:HB3	2.18	0.42
2:D:468:TYR:HB3	2:D:475:LEU:HB2	2.01	0.42
1:C:32:PRO:HB2	1:C:34:ILE:HG12	2.02	0.42
1:C:124:PHE:CE2	1:C:132:MET:HG2	2.55	0.42
1:A:124:PHE:CE2	1:A:132:MET:HG2	2.55	0.42
2:D:479:GLN:H	2:D:479:GLN:CD	2.22	0.42
2:B:468:TYR:HB3	2:B:475:LEU:HB2	2.01	0.42
1:A:326:LYS:HZ1	1:A:327:ILE:H	1.68	0.41
2:D:530:LEU:HD13	2:D:753:HIS:HB3	2.02	0.41
1:A:160:THR:HB	1:A:178:LEU:HB3	2.03	0.41
1:C:164:PRO:HG2	1:C:174:ALA:HB3	2.03	0.40
2:D:506:ILE:HB	2:D:672:MET:HB2	2.03	0.40
1:C:349:LEU:HD23	1:C:349:LEU:HA	1.99	0.40
2:B:501:GLU:HB2	2:B:776:LYS:HG3	2.03	0.40
2:B:631:VAL:CG1	2:B:632:ASP:N	2.83	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	356/375 (95%)	346 (97%)	10 (3%)	0	100	100
1	C	361/375 (96%)	349 (97%)	12 (3%)	0	100	100
2	B	396/413 (96%)	375 (95%)	21 (5%)	0	100	100
2	D	394/413 (95%)	374 (95%)	20 (5%)	0	100	100
All	All	1507/1576 (96%)	1444 (96%)	63 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/318 (95%)	289 (96%)	13 (4%)	29	53
1	C	307/318 (96%)	295 (96%)	12 (4%)	32	57
2	B	345/358 (96%)	318 (92%)	27 (8%)	12	24
2	D	344/358 (96%)	317 (92%)	27 (8%)	12	24
All	All	1298/1352 (96%)	1219 (94%)	79 (6%)	18	36

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	59	GLN

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Mol	Chain	Res	Type
1	A	64	ILE
1	A	95	ARG
1	A	116	ARG
1	A	132	MET
1	A	180	LEU
1	A	201	VAL
1	A	246	GLN
1	A	250	ILE
1	A	287	ILE
1	A	313	MET
1	A	354	GLN
2	B	466	LYS
2	B	479	GLN
2	B	512	VAL
2	B	530	LEU
2	B	542	MET
2	B	602	LEU
2	B	604	LEU
2	B	606	VAL
2	B	620	GLN
2	B	626	LEU
2	B	630	THR
2	B	643	ARG
2	B	644	GLU
2	B	657	VAL
2	B	674	THR
2	B	675	TYR
2	B	681	GLN
2	B	683	LYS
2	B	685	LYS
2	B	696	SER
2	B	718	LYS
2	B	731	LEU
2	B	745	THR
2	B	792	GLN
2	B	822	SER
2	B	836	ASP
2	B	837	SER
1	C	4	GLU
1	C	12	ASN
1	C	59	GLN
1	C	95	ARG

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Mol	Chain	Res	Type
1	C	116	ARG
1	C	132	MET
1	C	180	LEU
1	C	201	VAL
1	C	246	GLN
1	C	287	ILE
1	C	313	MET
1	C	354	GLN
2	D	466	LYS
2	D	479	GLN
2	D	491	VAL
2	D	512	VAL
2	D	526	SER
2	D	530	LEU
2	D	542	MET
2	D	563	LYS
2	D	570	GLN
2	D	595	LYS
2	D	604	LEU
2	D	616	THR
2	D	634	LYS
2	D	642	LEU
2	D	647	LEU
2	D	674	THR
2	D	675	TYR
2	D	685	LYS
2	D	696	SER
2	D	702	LEU
2	D	713	GLN
2	D	731	LEU
2	D	792	GLN
2	D	796	ASN
2	D	822	SER
2	D	837	SER
2	D	845	LYS

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

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 16 are monoatomic - leaving 15 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
3	LAB	C	401	-	28,29,29	0.29	0	30,41,41	1.13	4 (13%)
4	ATP	A	402	5	26,33,33	0.65	0	31,52,52	0.65	1 (3%)
6	SO4	D	1106	-	4,4,4	0.06	0	6,6,6	0.24	0
9	AZI	D	1113	-	0,2,2	-	-	0,1,1	-	-
9	AZI	D	1114	-	0,2,2	-	-	0,1,1	-	-
3	LAB	A	401	-	28,29,29	0.28	0	30,41,41	1.16	4 (13%)
9	AZI	D	1115	8	0,2,2	-	-	0,1,1	-	-
7	3AT	B	1101	8,5	25,32,32	0.68	0	28,50,50	0.81	1 (3%)
7	3AT	D	1101	8,5	25,32,32	0.75	0	28,50,50	0.87	1 (3%)
9	AZI	D	1110	8	0,2,2	-	-	0,1,1	-	-
9	AZI	D	1111	8	0,2,2	-	-	0,1,1	-	-
6	SO4	C	405	-	4,4,4	0.12	0	6,6,6	0.12	0
6	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.23	0
9	AZI	D	1112	8	0,2,2	-	-	0,1,1	-	-
4	ATP	C	402	8,5	26,33,33	0.65	0	31,52,52	0.68	1 (3%)

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
3	LAB	C	401	-	-	3/21/49/49	0/2/3/3
4	ATP	A	402	5	-	3/18/38/38	0/3/3/3
3	LAB	A	401	-	-	3/21/49/49	0/2/3/3
7	3AT	B	1101	8,5	-	6/18/34/34	0/3/3/3
7	3AT	D	1101	8,5	-	6/18/34/34	0/3/3/3
4	ATP	C	402	8,5	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	LAB	C10-C9-C8	3.52	119.81	113.95
3	A	401	LAB	C10-C9-C8	3.49	119.76	113.95
3	A	401	LAB	O3-C15-C16	2.95	108.03	104.25
3	C	401	LAB	O3-C15-C16	2.89	107.96	104.25
3	C	401	LAB	C3-C2-C1	2.60	133.89	127.46
3	A	401	LAB	C3-C2-C1	2.50	133.64	127.46
4	C	402	ATP	C5-C6-N6	2.36	123.94	120.35
7	B	1101	3AT	C5-C6-N6	2.30	123.85	120.35
3	A	401	LAB	C14-C15-C16	-2.29	109.28	113.75
7	D	1101	3AT	C5-C6-N6	2.22	123.73	120.35
3	C	401	LAB	C14-C15-C16	-2.07	109.72	113.75
4	A	402	ATP	C5-C6-N6	2.06	123.48	120.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	ATP	C5'-O5'-PA-O1A
4	C	402	ATP	C5'-O5'-PA-O1A
7	B	1101	3AT	PB-O3B-PG-O2G
7	B	1101	3AT	O4'-C4'-C5'-O5'
7	B	1101	3AT	C3'-C4'-C5'-O5'
7	D	1101	3AT	PB-O3B-PG-O2G
7	D	1101	3AT	O4'-C4'-C5'-O5'
7	D	1101	3AT	C3'-C4'-C5'-O5'
7	D	1101	3AT	C4'-C5'-O5'-PA
4	A	402	ATP	C5'-O5'-PA-O3A
4	C	402	ATP	C5'-O5'-PA-O3A
4	A	402	ATP	PG-O3B-PB-O1B
4	C	402	ATP	PG-O3B-PB-O1B

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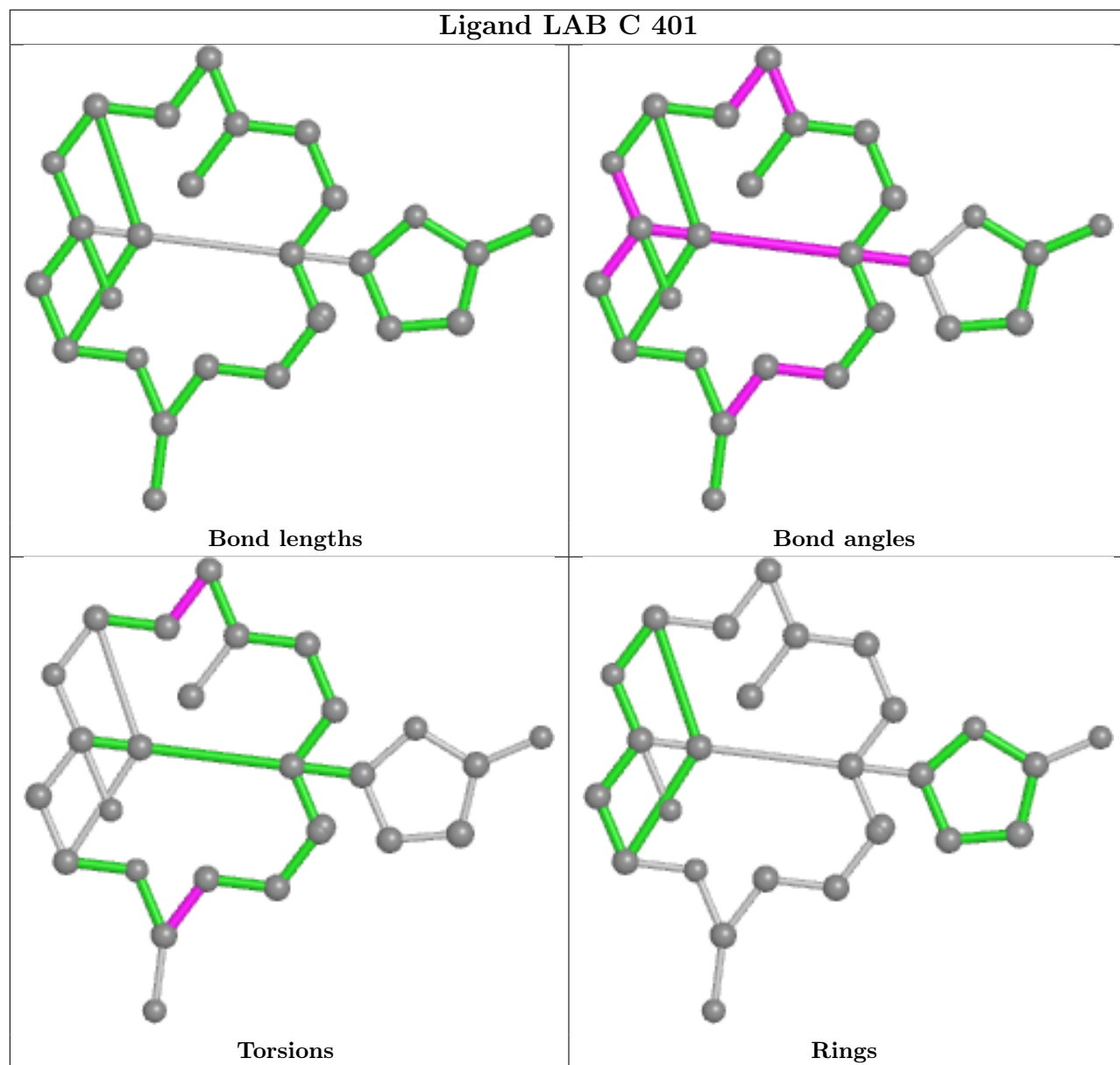
Mol	Chain	Res	Type	Atoms
7	B	1101	3AT	C4'-C5'-O5'-PA
3	A	401	LAB	O2-C1-C2-C3
3	C	401	LAB	O2-C1-C2-C3
7	B	1101	3AT	PB-O3B-PG-O3G
7	B	1101	3AT	PA-O3A-PB-O2B
7	D	1101	3AT	PA-O3A-PB-O1B
7	D	1101	3AT	PA-O3A-PB-O2B
3	A	401	LAB	O1-C1-C2-C3
3	A	401	LAB	C11-C10-C9-C8
3	C	401	LAB	C11-C10-C9-C8
3	C	401	LAB	O1-C1-C2-C3

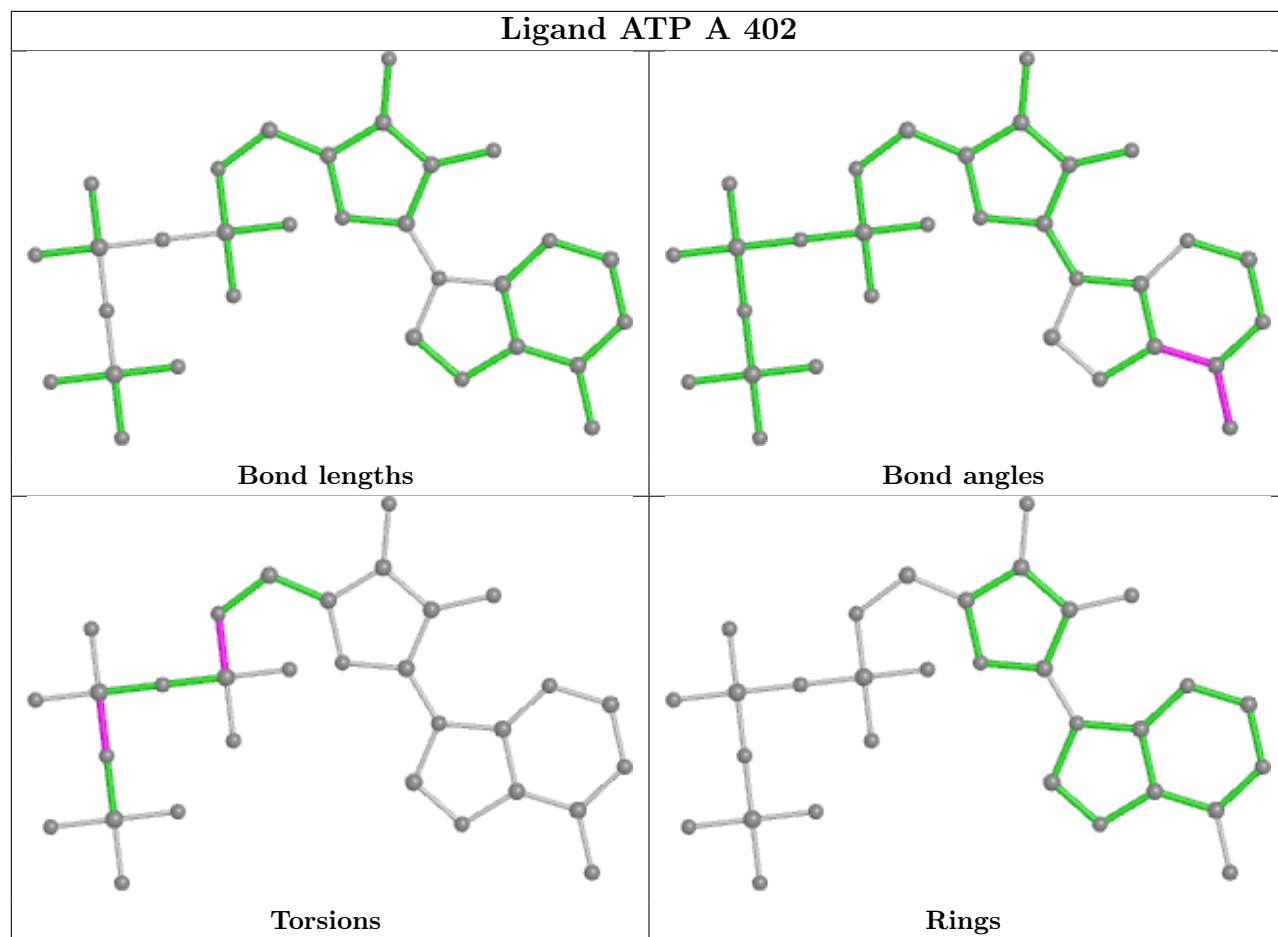
There are no ring outliers.

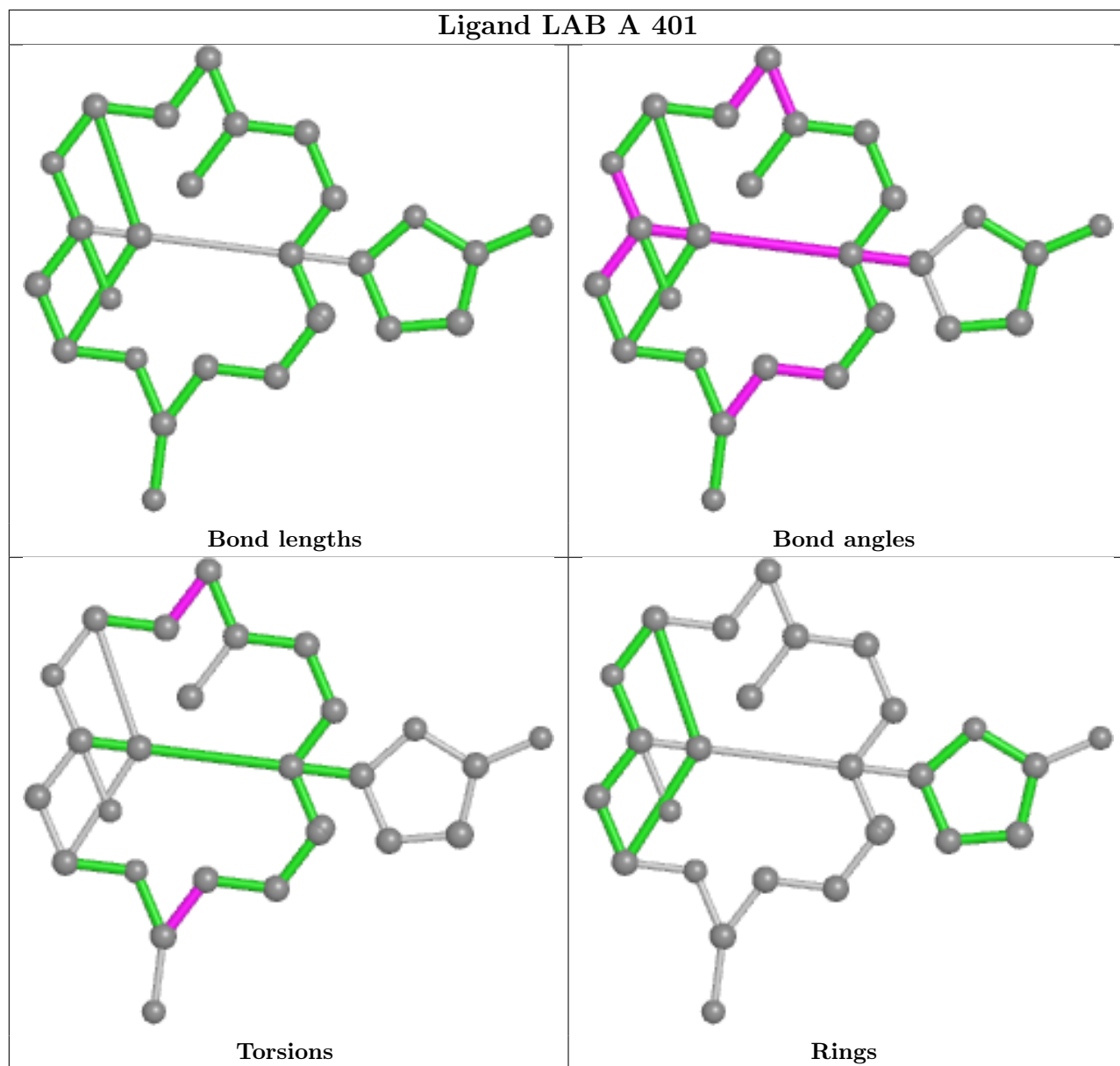
2 monomers are involved in 2 short contacts:

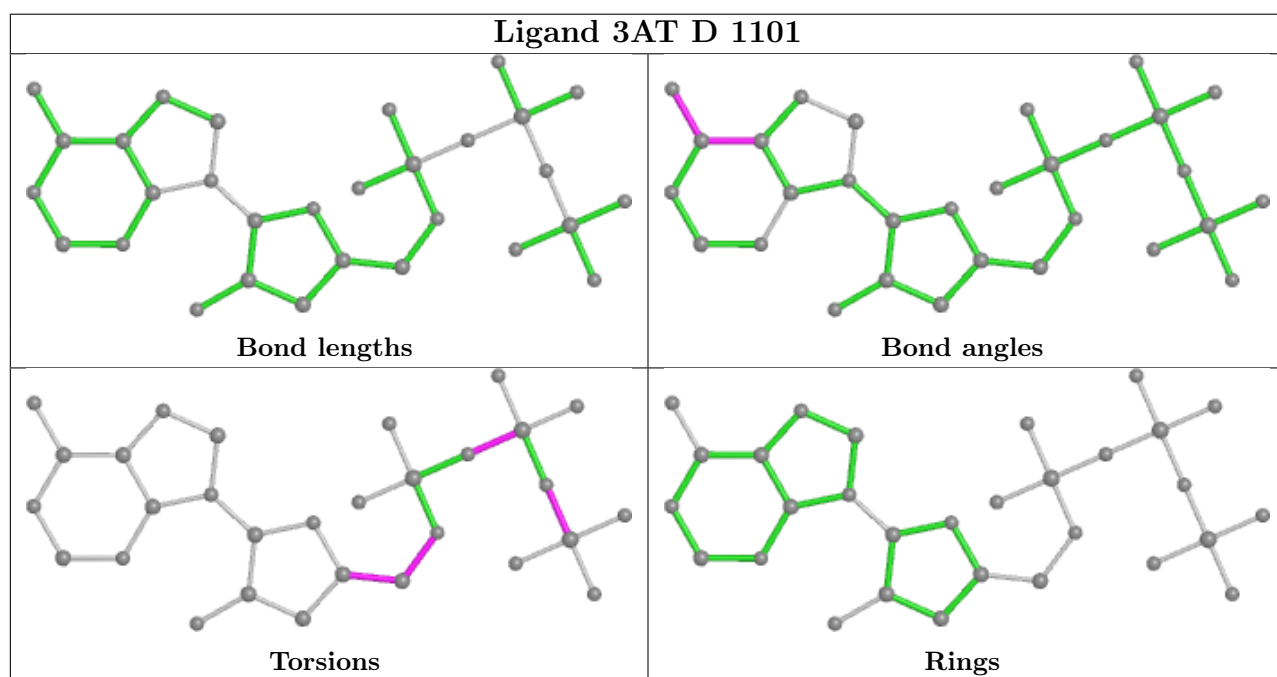
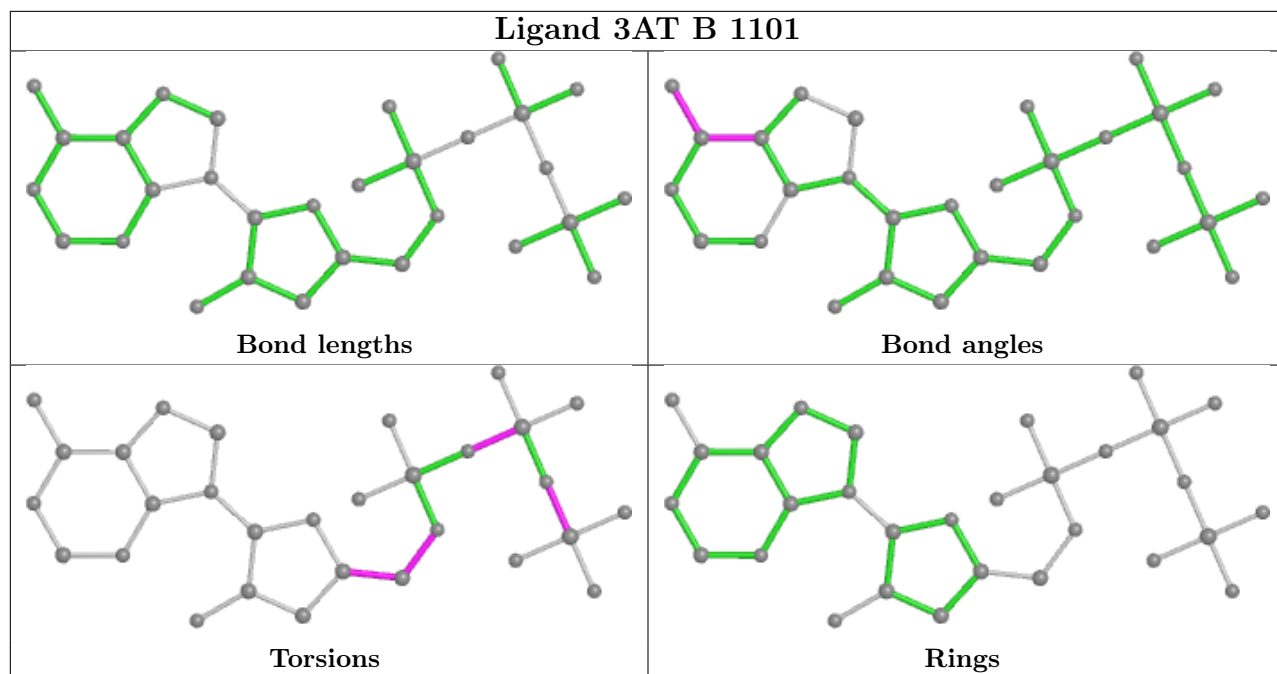
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	LAB	1	0
3	A	401	LAB	1	0

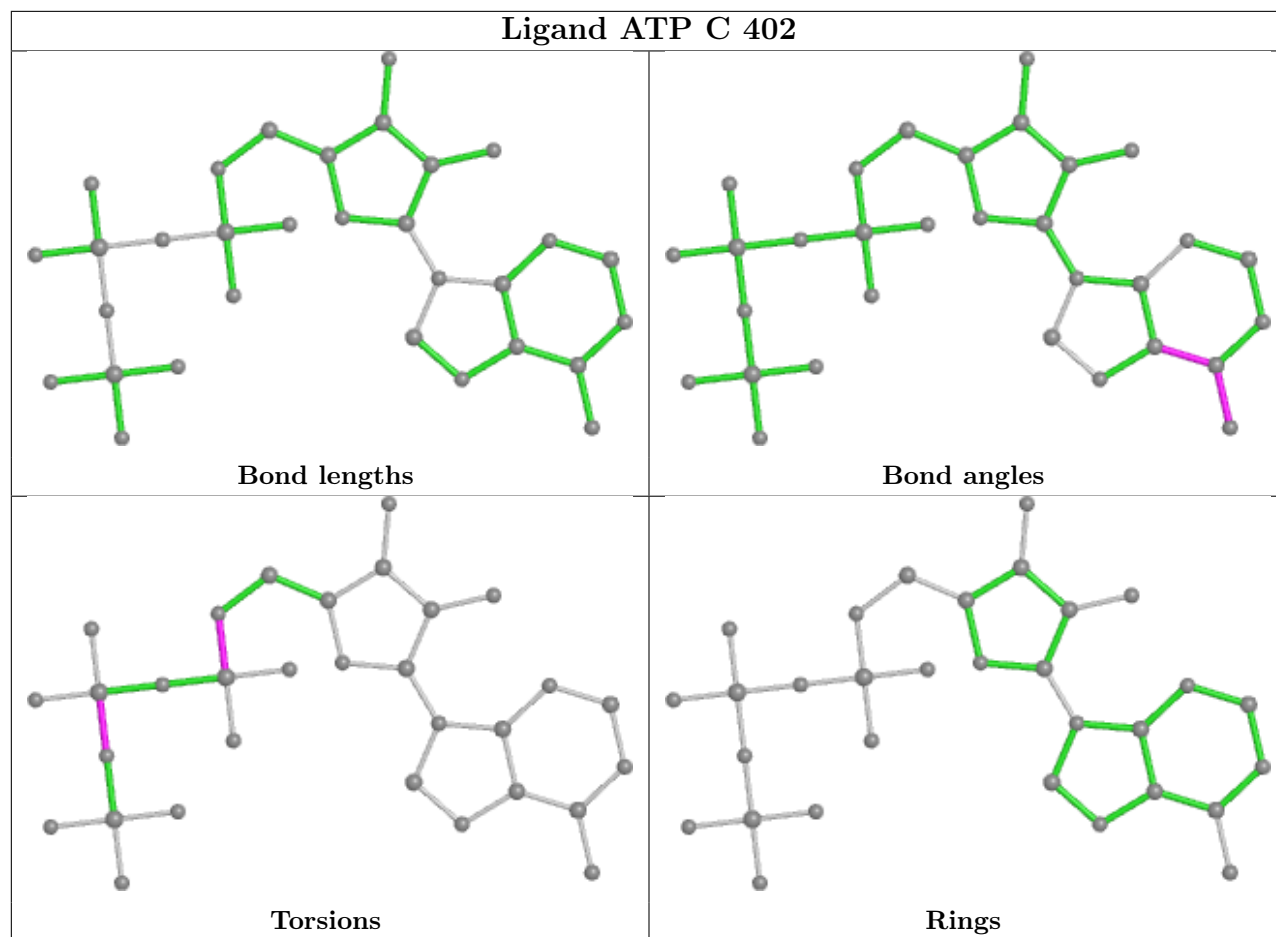
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	360/375 (96%)	0.57	17 (4%) 31 33	56, 79, 112, 133	0
1	C	364/375 (97%)	0.89	47 (12%) 3 3	67, 96, 139, 151	0
2	B	398/413 (96%)	0.60	32 (8%) 12 12	57, 77, 120, 128	0
2	D	396/413 (95%)	0.56	27 (6%) 17 17	52, 74, 106, 120	0
All	All	1518/1576 (96%)	0.65	123 (8%) 12 12	52, 81, 120, 151	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	350	SER	8.2
1	A	38	PRO	7.2
1	C	39[A]	ARG	6.9
2	B	619	ASP	5.9
1	A	350	SER	5.7
1	C	43	VAL	5.4
2	B	607	ASP	5.0
1	C	53	TYR	4.9
1	A	64	ILE	4.8
1	C	370	VAL	4.7
1	C	236	LEU	4.6
2	D	604	LEU	4.4
1	C	68	LYS	4.3
2	B	704	PRO	4.2
1	C	352	PHE	4.2
2	D	480	HIS	4.1
1	A	40	HIS	4.1
1	C	44	MET	4.1
1	C	359	LYS	4.0
2	B	706	TYR	4.0
1	A	65	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	67	LEU	3.9
2	B	636	LEU	3.9
2	B	625	PHE	3.8
1	C	364	GLU	3.8
1	A	39	ARG	3.8
1	A	354	GLN	3.8
2	B	637	TRP	3.8
1	A	49	GLN	3.8
1	C	49	GLN	3.7
1	C	235	SER	3.7
1	C	34	ILE	3.6
1	C	42	GLY	3.6
1	C	328	LYS	3.6
1	C	59	GLN	3.6
2	D	603	GLU	3.6
2	B	611	TYR	3.5
2	B	602	LEU	3.5
2	B	631	VAL	3.5
2	B	699	TYR	3.5
1	A	328	LYS	3.3
2	B	702	LEU	3.3
1	A	53	TYR	3.3
2	D	473	LEU	3.2
2	B	620	GLN	3.2
1	C	41	GLN	3.2
2	D	700	GLU	3.1
2	D	611	TYR	3.1
2	D	786	GLU	3.1
2	D	602	LEU	3.0
1	C	69	TYR	3.0
2	D	474	VAL	3.0
1	C	349	LEU	3.0
2	D	781	ASP	2.9
2	D	715	LEU	2.9
1	C	360	GLN	2.9
2	B	646	GLU	2.8
1	C	294	TYR	2.8
1	C	327	ILE	2.8
2	D	606	VAL	2.8
1	C	63	GLY	2.8
1	C	326	LYS	2.8
2	B	629	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	232	SER	2.7
1	C	125	GLU	2.7
1	A	356	TRP	2.7
1	C	353	GLN	2.7
1	C	354	GLN	2.7
2	D	637	TRP	2.7
2	B	707	LYS	2.6
2	B	697	VAL	2.6
2	D	697	VAL	2.6
1	C	64	ILE	2.6
2	D	625	PHE	2.6
1	A	50	LYS	2.6
2	B	621	THR	2.6
2	D	702	LEU	2.6
1	A	37	ARG	2.6
2	B	589	ILE	2.5
2	D	710	TYR	2.5
2	D	557	ALA	2.5
1	C	84	LYS	2.5
1	C	371	HIS	2.5
2	B	786	GLU	2.5
1	C	362	TYR	2.5
2	B	469	GLN	2.4
2	D	631	VAL	2.4
2	D	479	GLN	2.4
2	B	606	VAL	2.4
2	D	589	ILE	2.4
1	C	231	ALA	2.4
1	C	234	SER	2.4
2	D	605	ASP	2.4
1	C	142	LEU	2.4
1	C	363	ASP	2.3
1	A	132	MET	2.3
1	C	52	SER	2.3
2	B	835	LEU	2.3
1	C	289	ILE	2.3
2	D	784	LEU	2.3
1	C	292	ASP	2.3
1	C	37	ARG	2.2
2	B	615	ALA	2.2
2	B	635	GLU	2.2
2	B	612	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	327	ILE	2.2
2	B	791	ILE	2.2
1	C	202	THR	2.2
2	D	476	GLU	2.2
2	B	604	LEU	2.2
2	D	780	ASP	2.1
1	C	36	GLY	2.1
1	C	250	ILE	2.1
1	C	201	VAL	2.1
1	C	77	THR	2.1
1	A	367	PRO	2.1
1	A	95	ARG	2.1
2	D	475	LEU	2.1
2	B	617	ASN	2.1
2	B	601	PRO	2.1
2	B	466	LYS	2.0
2	B	647	LEU	2.0
2	D	861	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	C	405	5/5	0.43	0.93	80,80,80,80	5
6	SO4	A	404	5/5	0.77	0.45	83,83,83,83	5
9	AZI	D	1112	3/3	0.82	0.28	73,73,73,73	0
8	MN	C	404[B]	1/1	0.91	0.26	81,81,81,81	1
8	MN	D	1109	1/1	0.91	0.21	87,87,87,87	0

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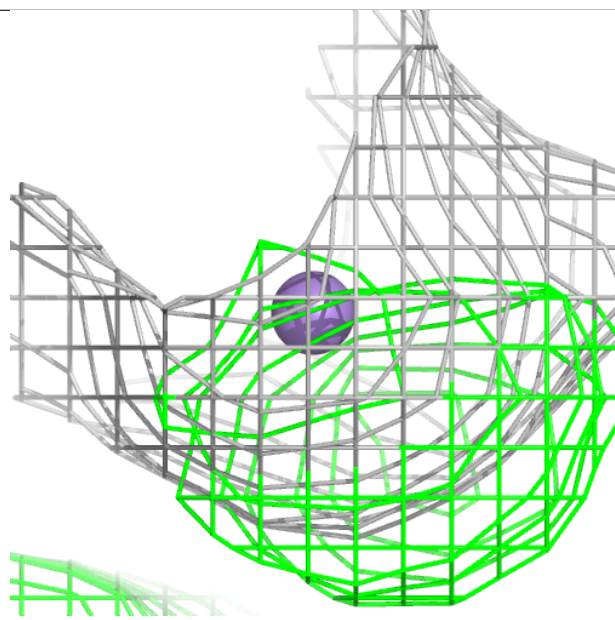
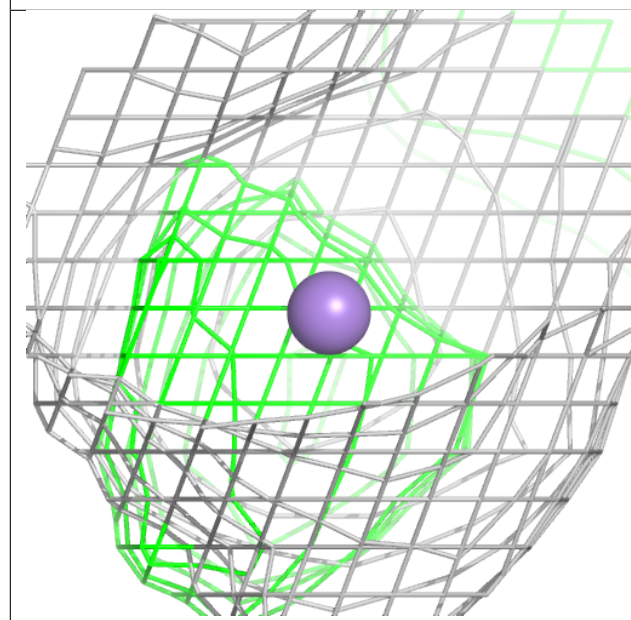
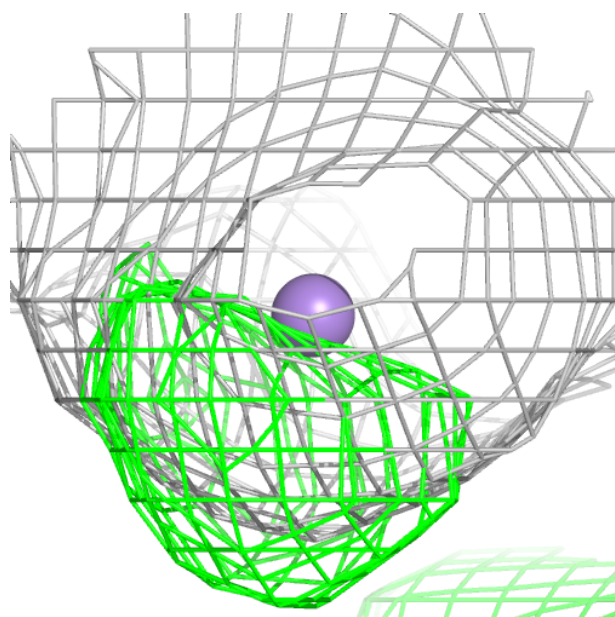
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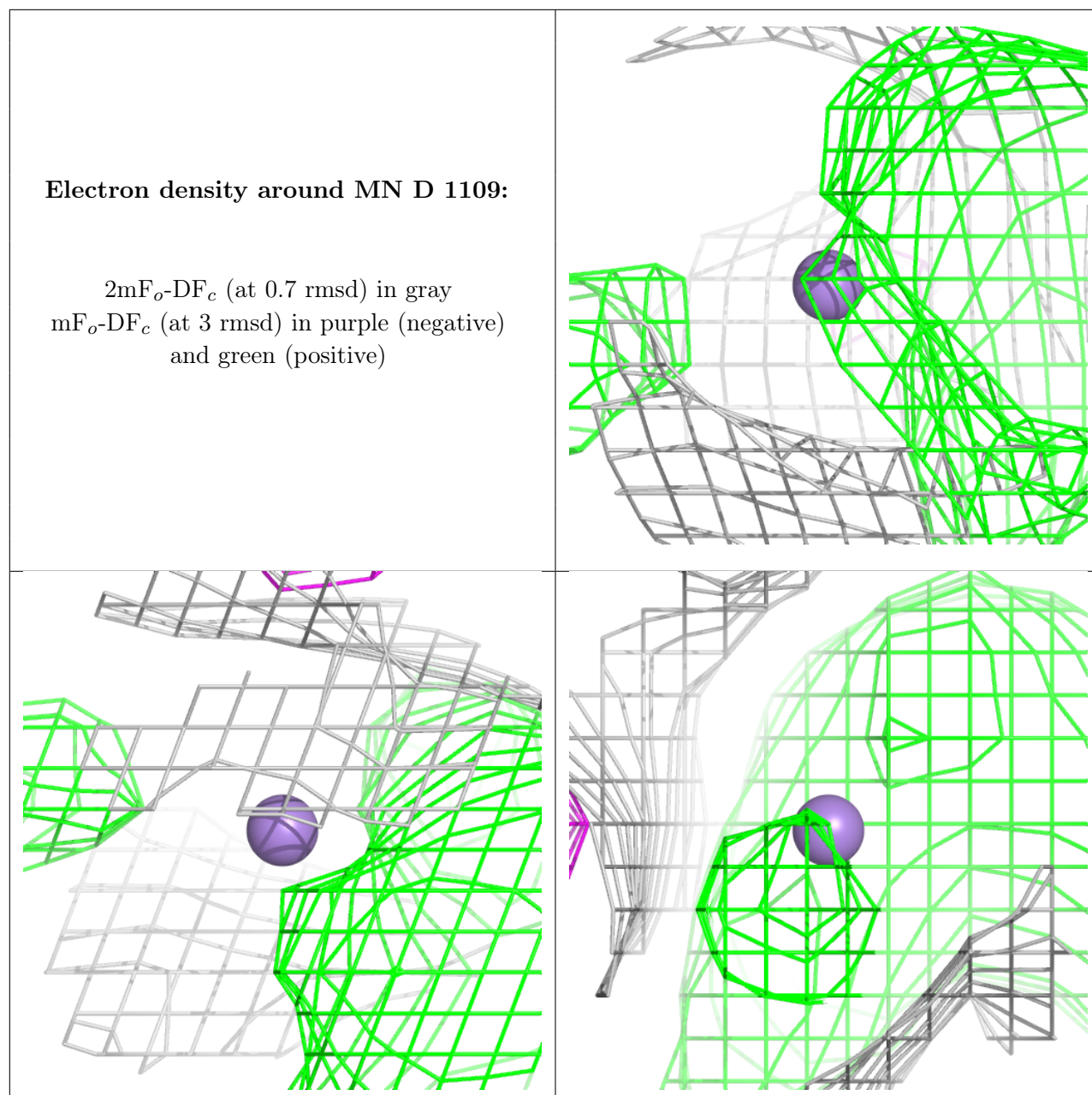
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	C	403[A]	1/1	0.91	0.26	81,81,81,81	1
8	MN	D	1102[B]	1/1	0.92	0.14	66,66,66,66	1
5	MG	D	1103[A]	1/1	0.92	0.14	66,66,66,66	1
3	LAB	C	401	27/27	0.92	0.23	101,103,104,104	0
5	MG	D	1105[A]	1/1	0.93	0.20	67,67,67,67	1
8	MN	D	1104[B]	1/1	0.93	0.20	67,67,67,67	1
9	AZI	D	1114	3/3	0.94	0.46	71,71,71,71	0
3	LAB	A	401	27/27	0.95	0.20	81,84,88,89	0
9	AZI	D	1110	3/3	0.95	0.31	67,67,67,67	0
9	AZI	D	1111	3/3	0.95	0.28	60,60,61,62	0
4	ATP	C	402	31/31	0.95	0.17	81,83,86,87	0
8	MN	D	1107	1/1	0.95	0.20	87,87,87,87	0
6	SO4	D	1106	5/5	0.96	0.24	61,61,61,62	5
7	3AT	B	1101	30/30	0.96	0.18	66,68,70,70	0
8	MN	B	1104[B]	1/1	0.96	0.17	62,62,62,62	1
9	AZI	D	1113	3/3	0.96	0.44	66,66,66,66	0
5	MG	B	1105[A]	1/1	0.96	0.17	62,62,62,62	1
9	AZI	D	1115	3/3	0.96	0.25	65,65,65,65	0
10	CL	D	1117	1/1	0.96	0.39	77,77,77,77	0
7	3AT	D	1101	30/30	0.97	0.20	55,66,69,69	0
8	MN	D	1108	1/1	0.97	0.26	80,80,80,80	0
5	MG	A	403	1/1	0.98	0.17	54,54,54,54	0
10	CL	D	1116	1/1	0.98	0.33	80,80,80,80	0
4	ATP	A	402	31/31	0.98	0.17	59,64,72,73	0
8	MN	B	1102[B]	1/1	0.99	0.17	64,64,64,64	1
5	MG	B	1103[A]	1/1	0.99	0.17	64,64,64,64	1

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

Electron density around MN C 404 (B):

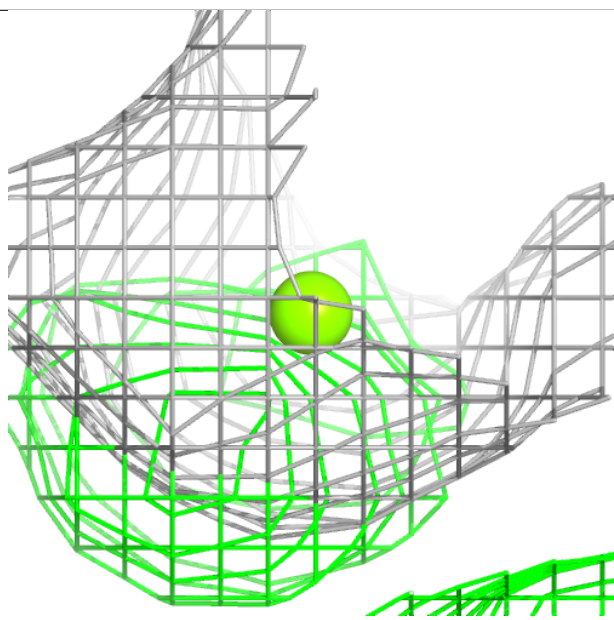
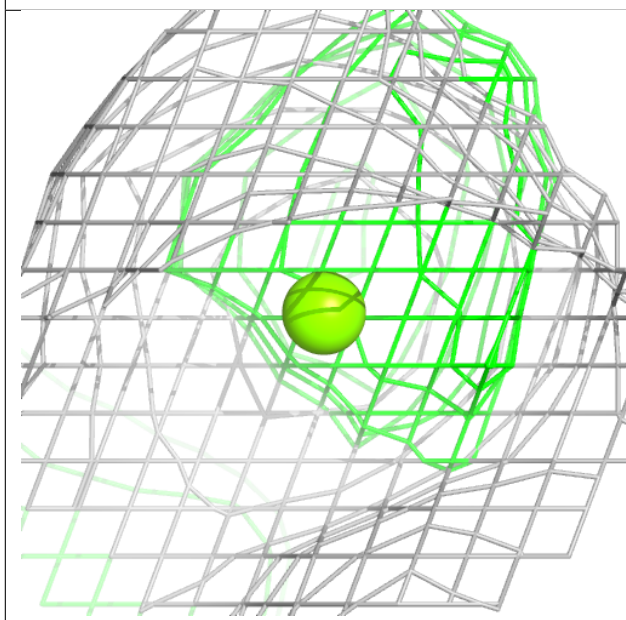
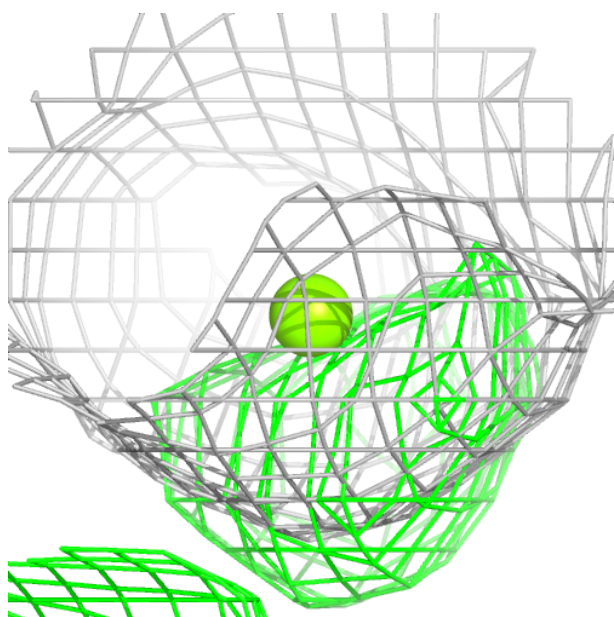
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





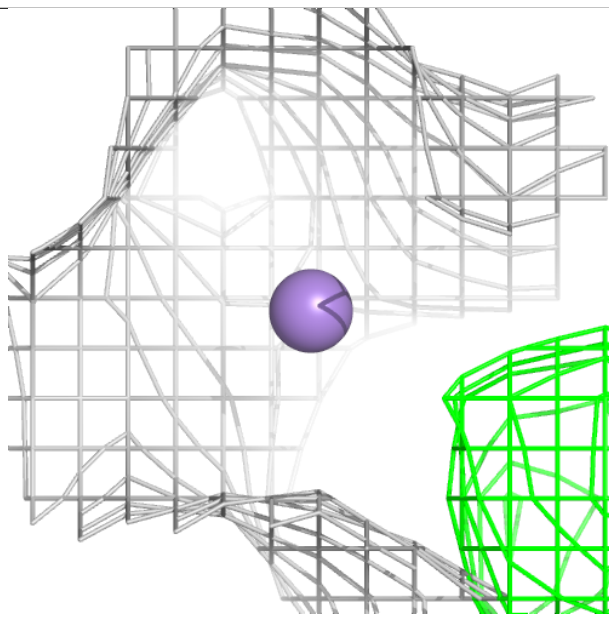
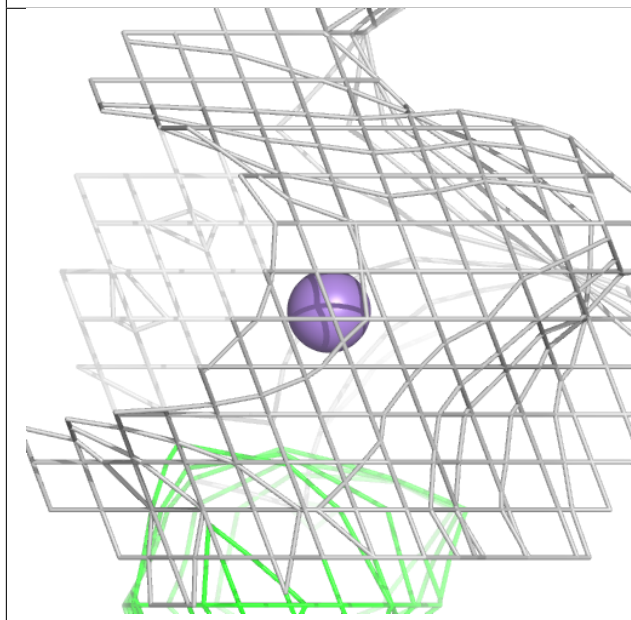
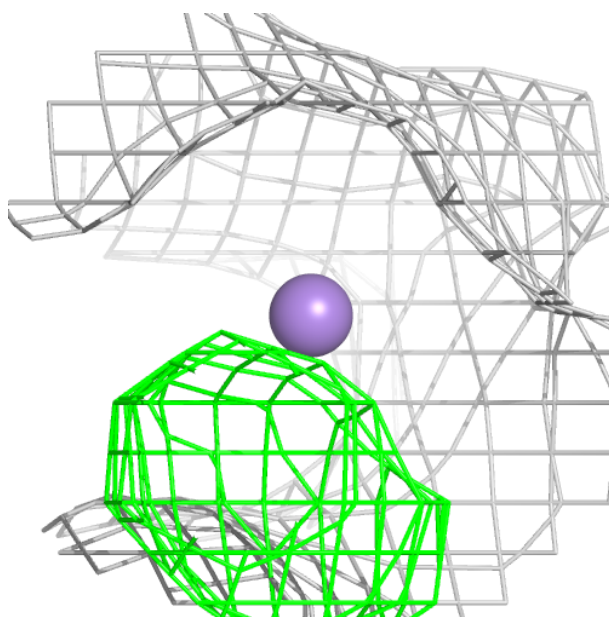
Electron density around MG C 403 (A):

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



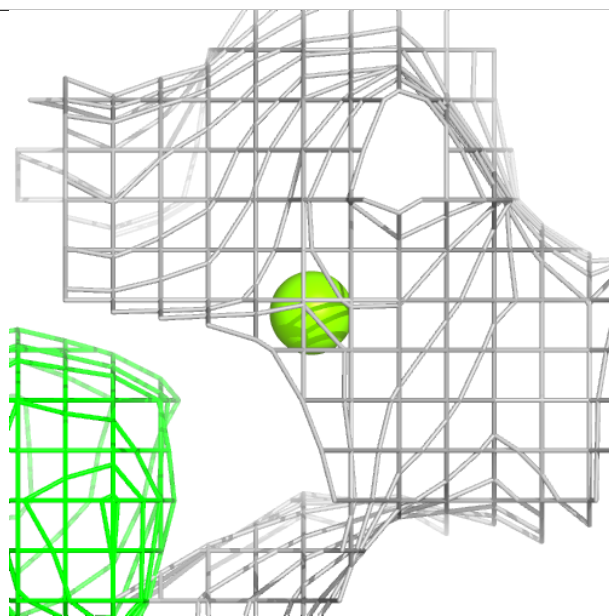
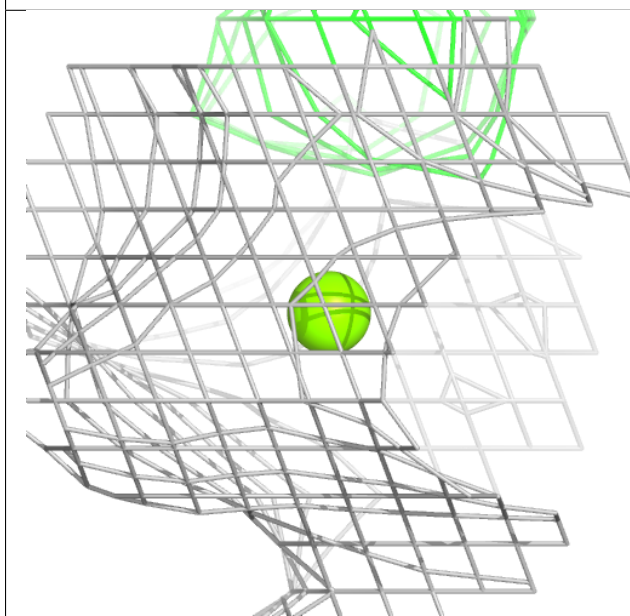
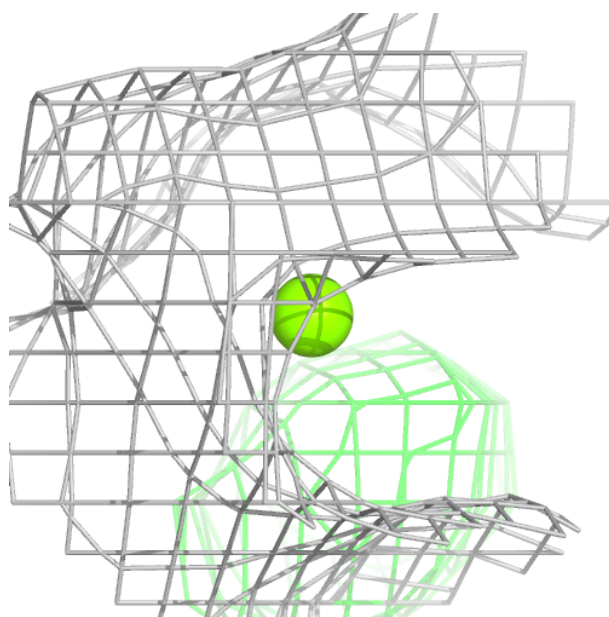
Electron density around MN D 1102 (B):

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



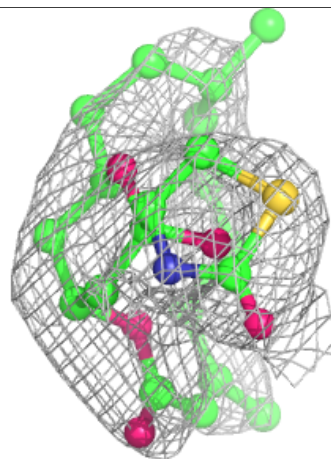
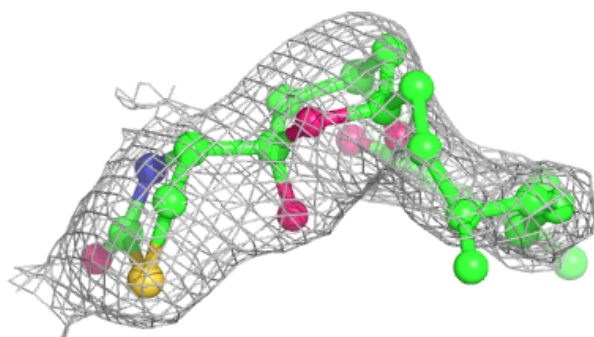
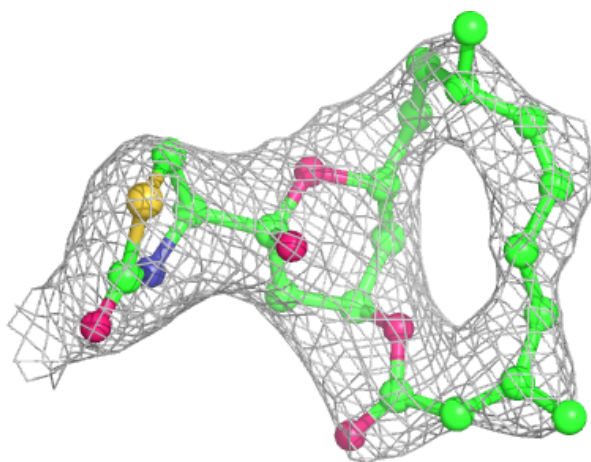
Electron density around MG D 1103 (A):

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



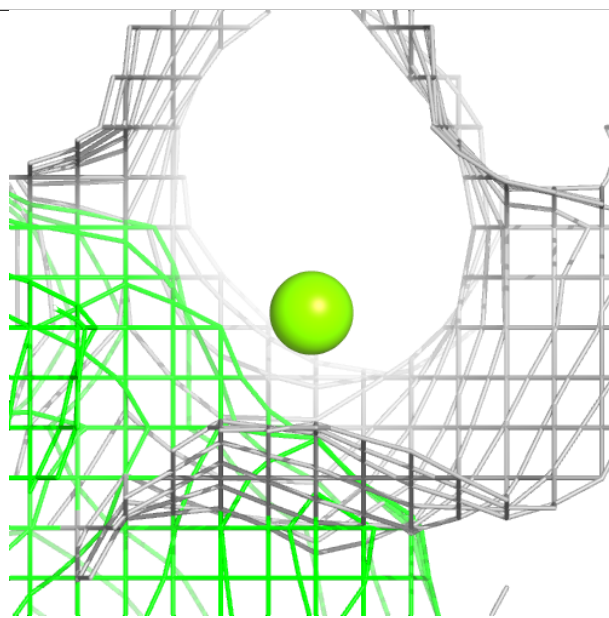
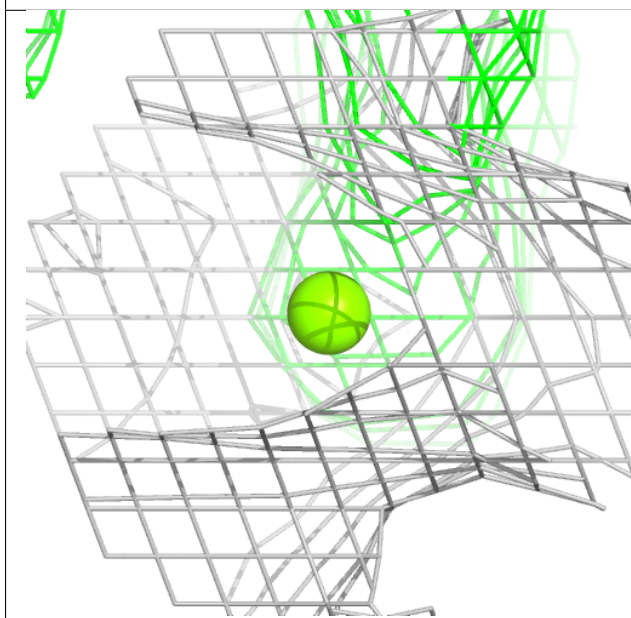
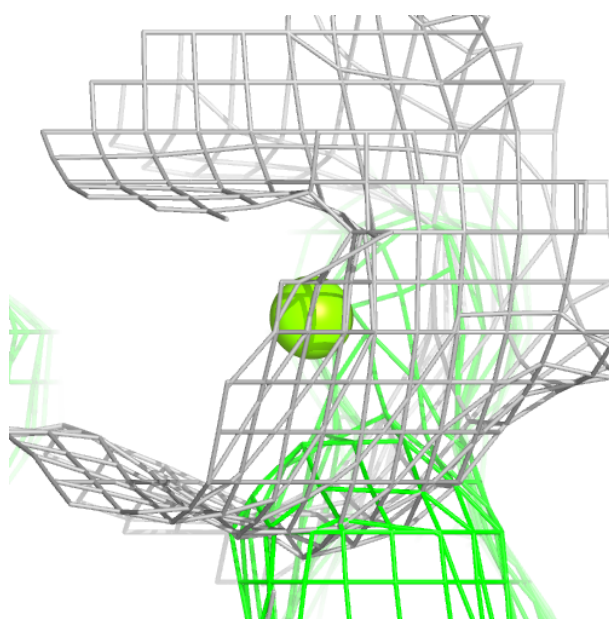
Electron density around LAB C 401:

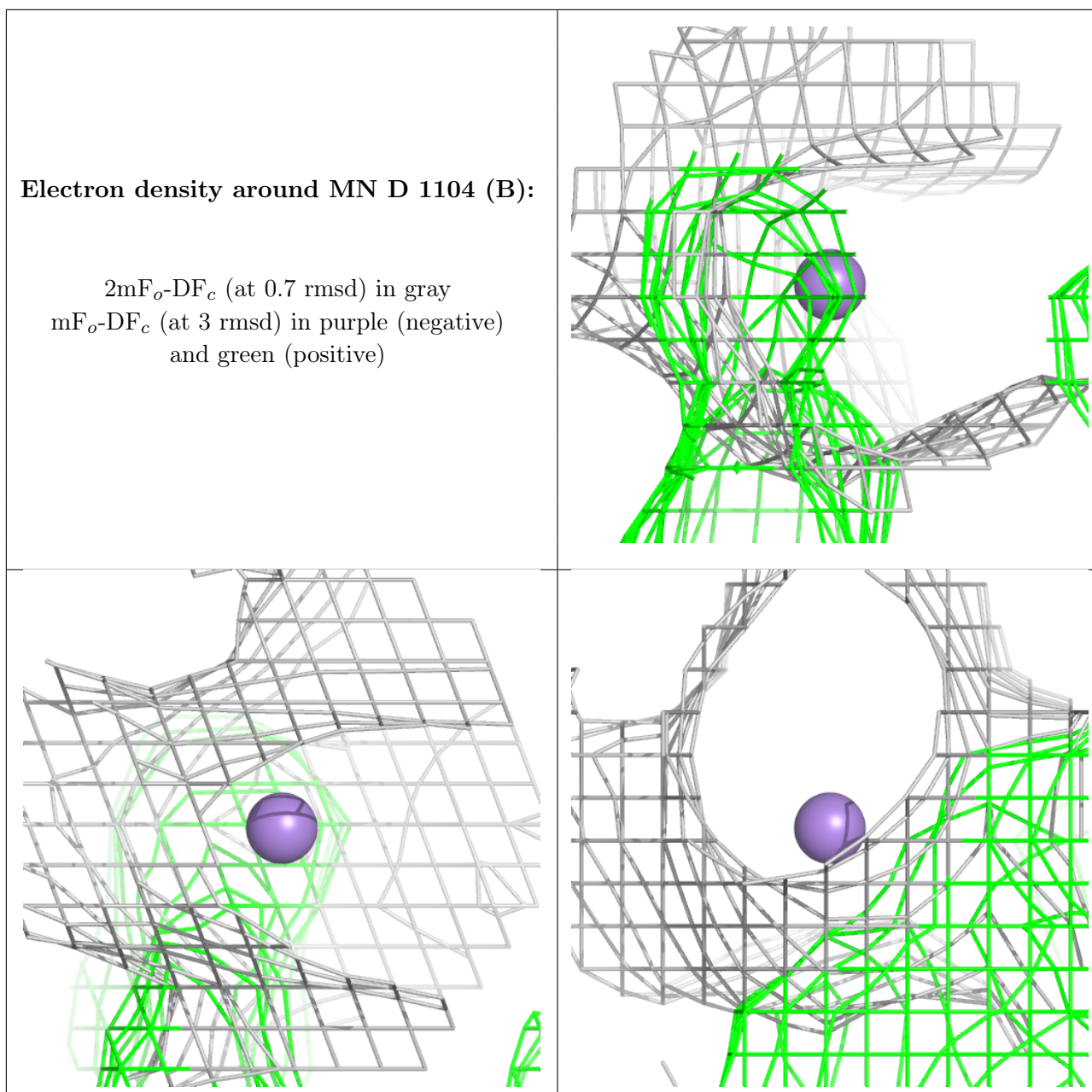
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 1105 (A):

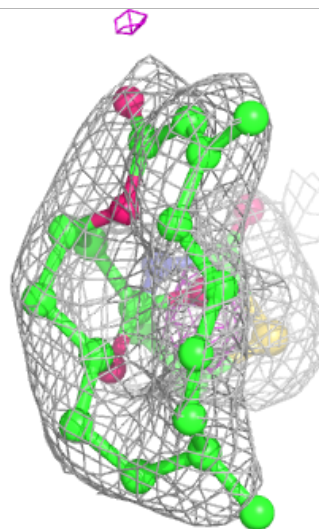
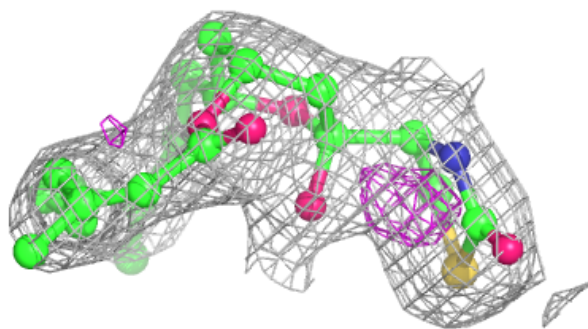
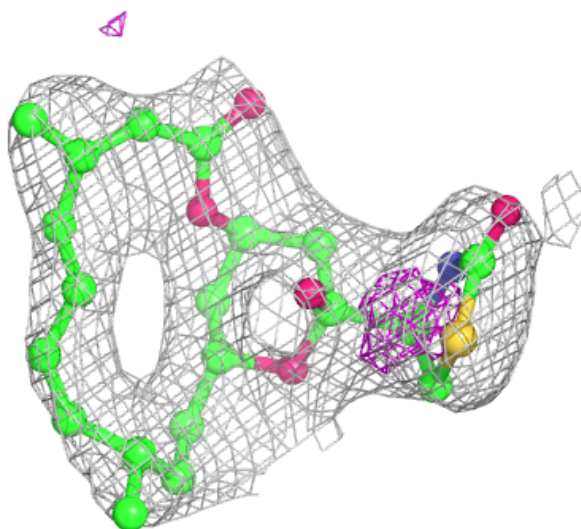
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





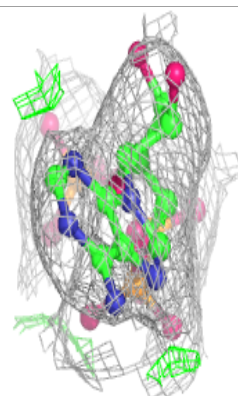
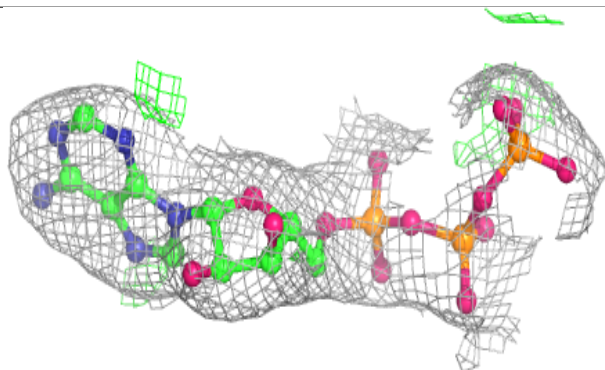
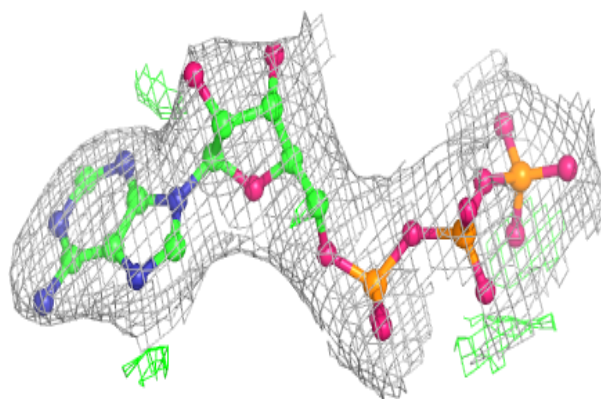
Electron density around LAB A 401:

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



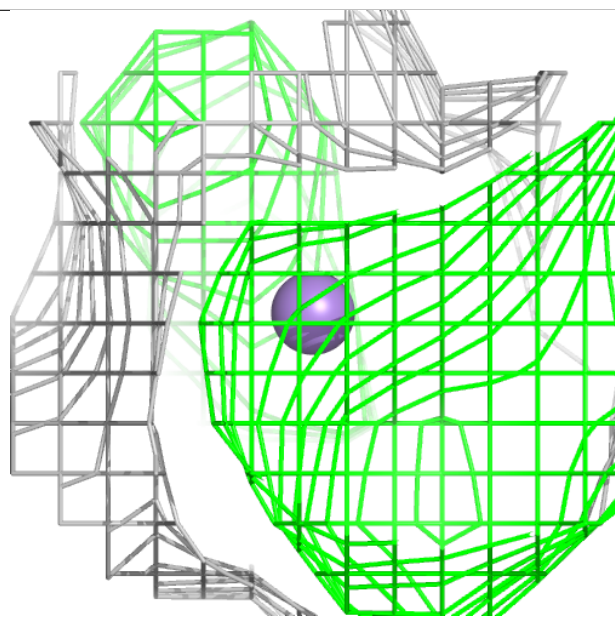
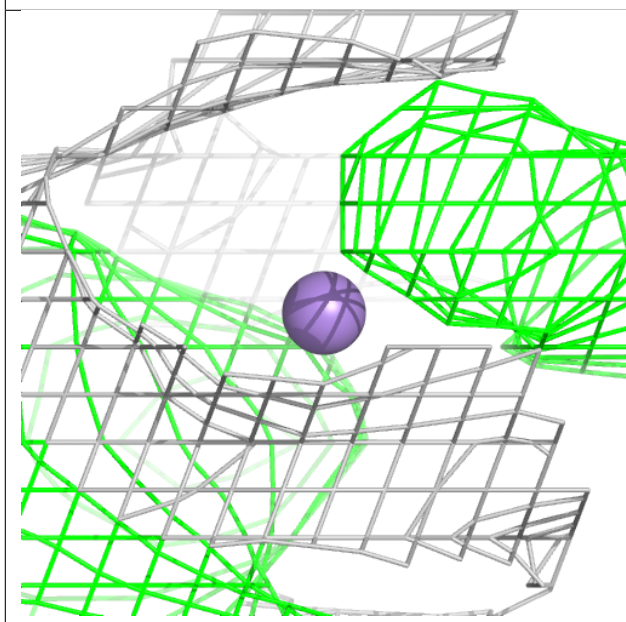
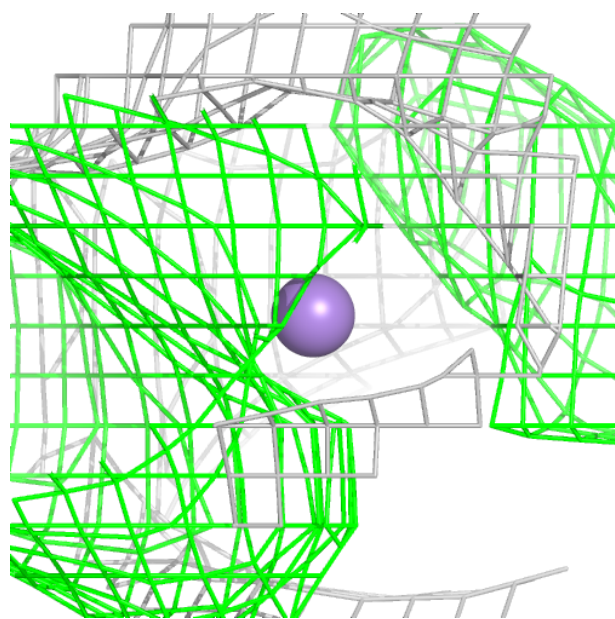
Electron density around ATP C 402:

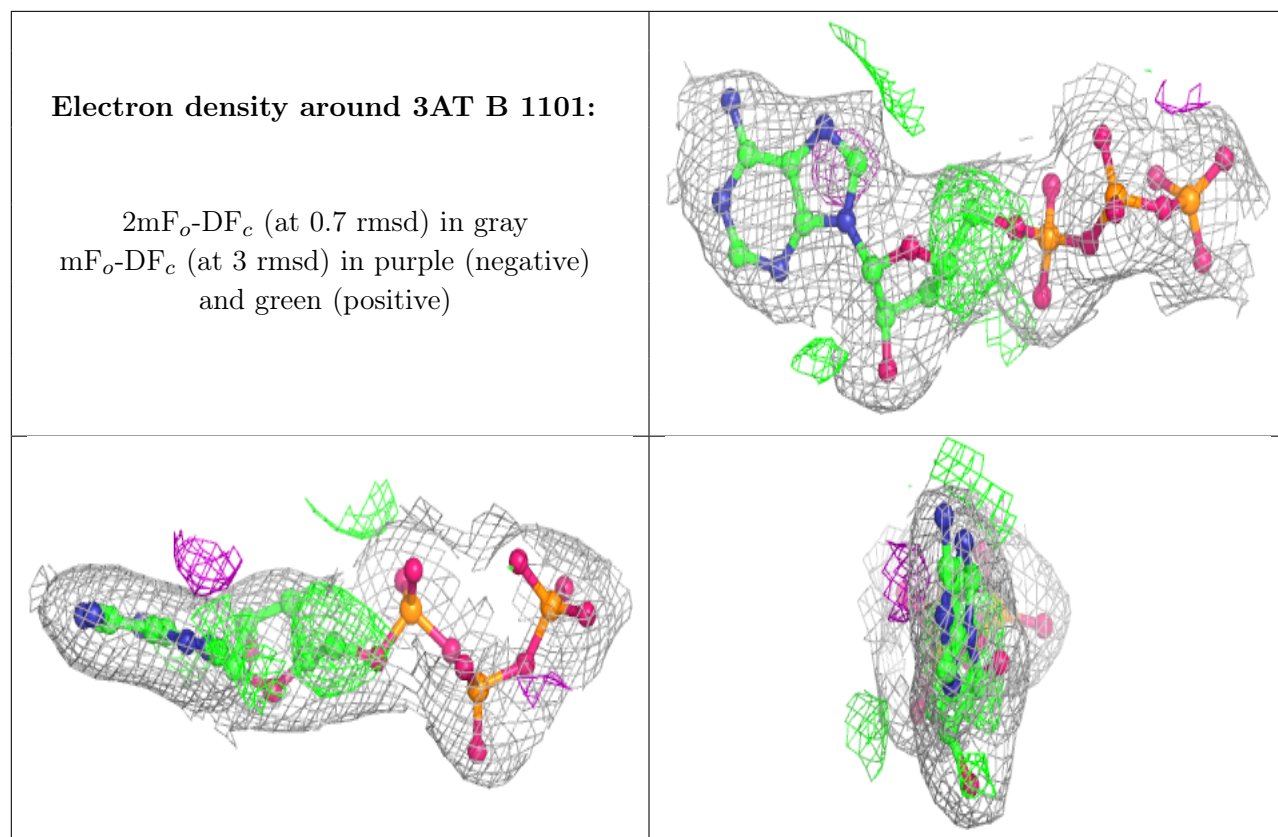
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

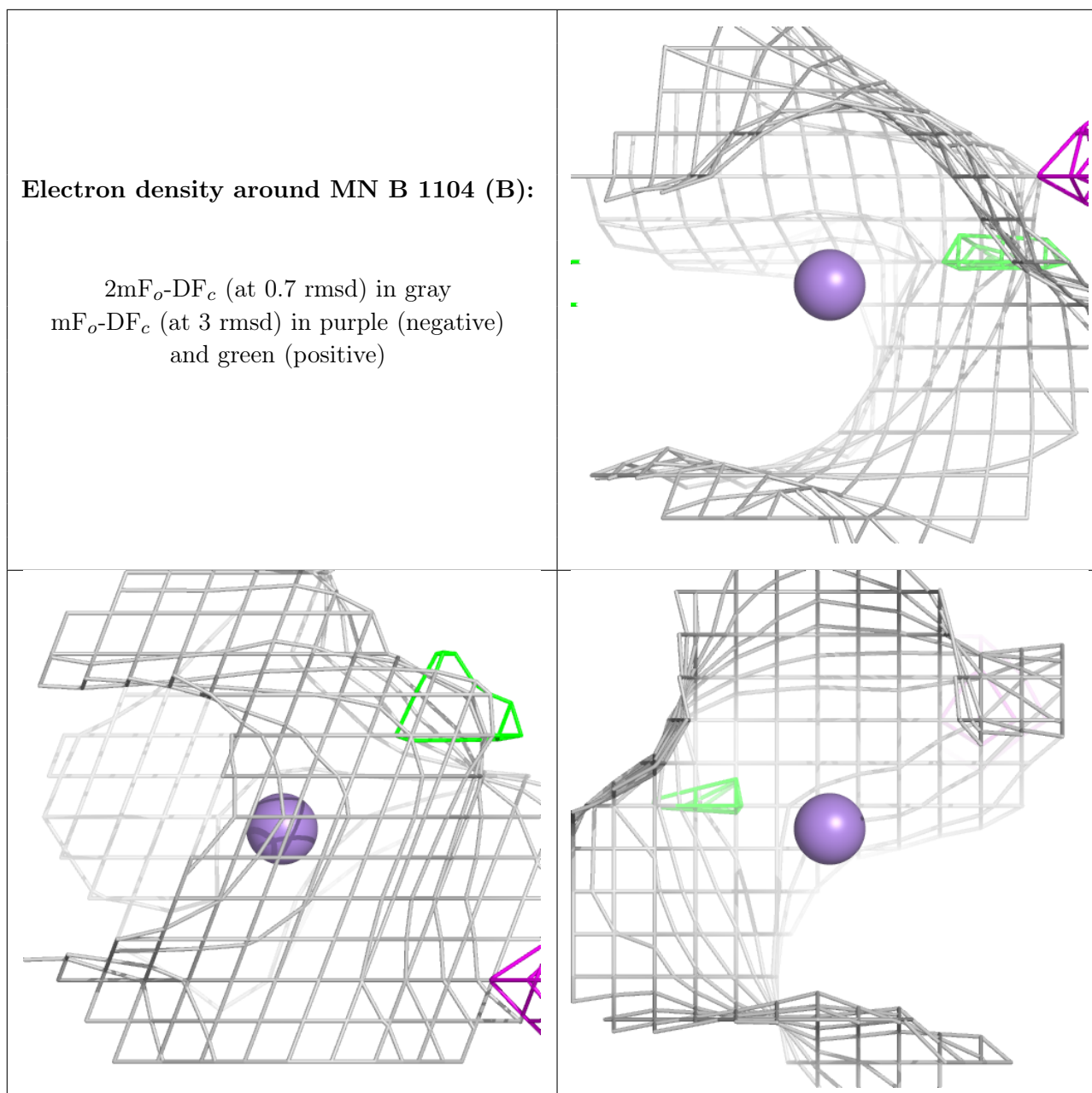


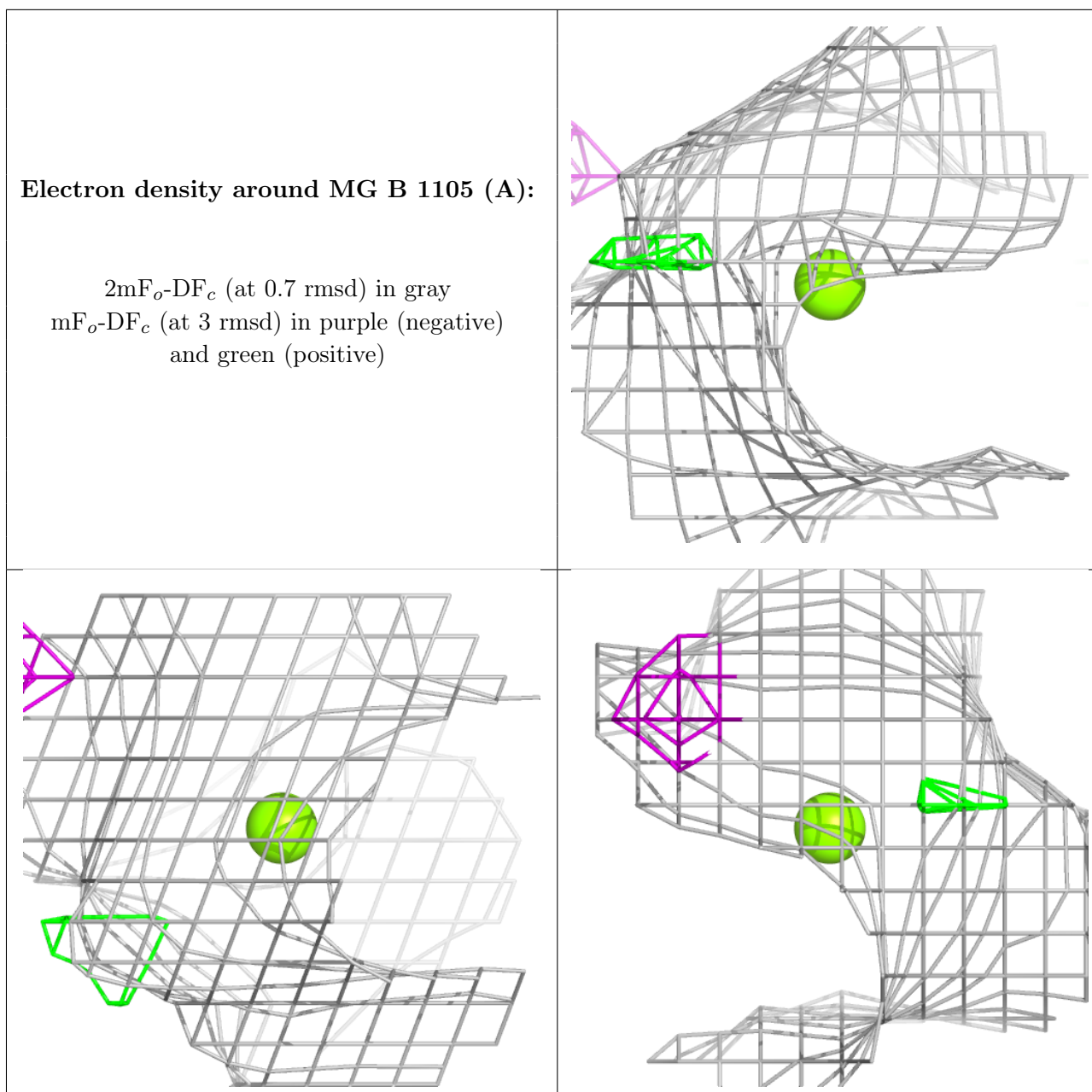
Electron density around MN D 1107:

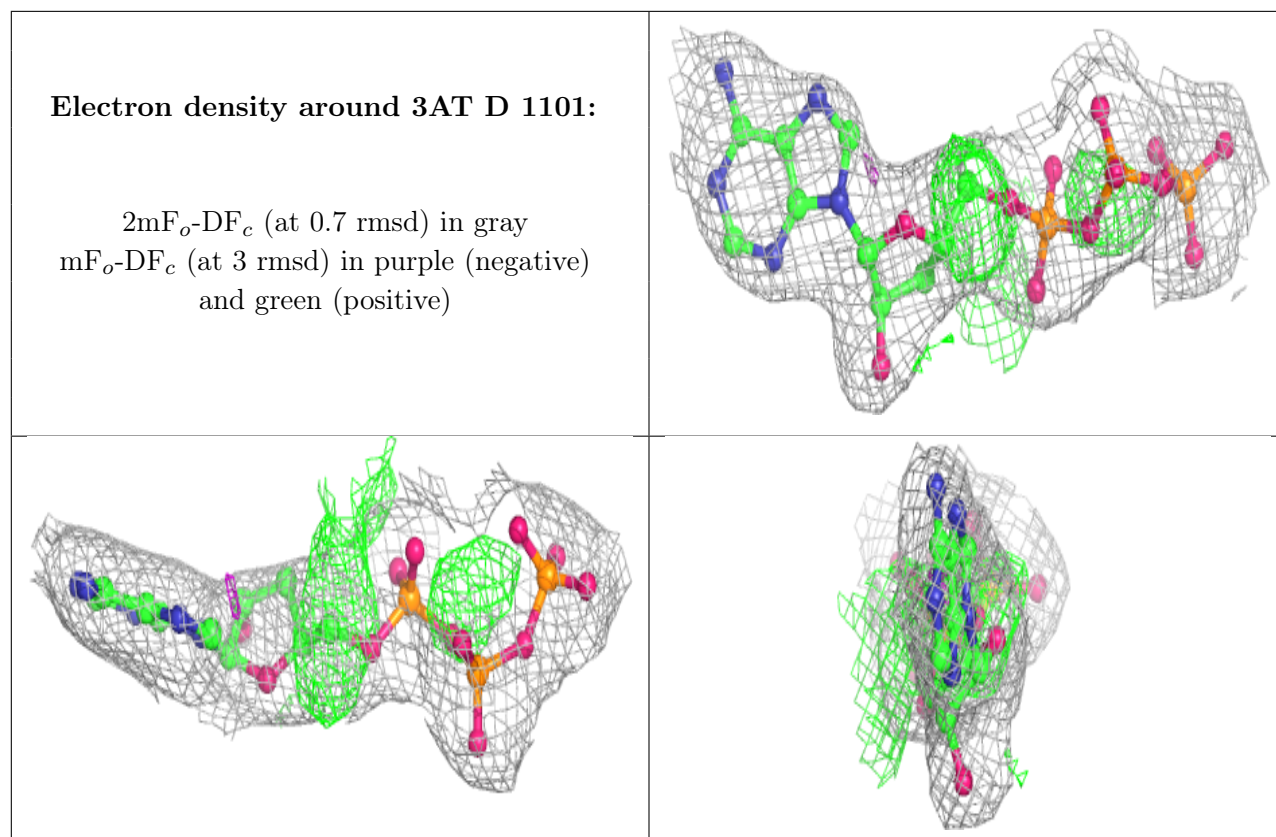
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





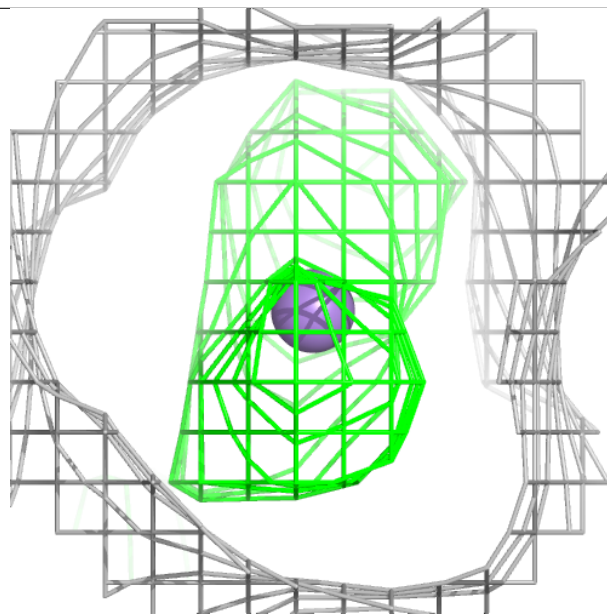
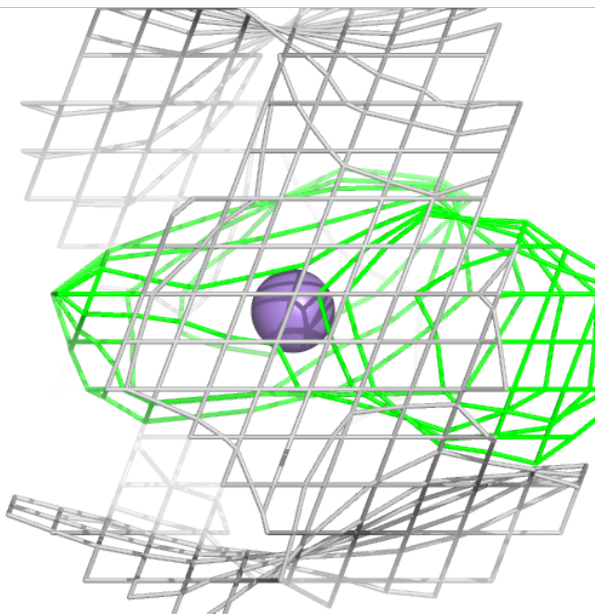
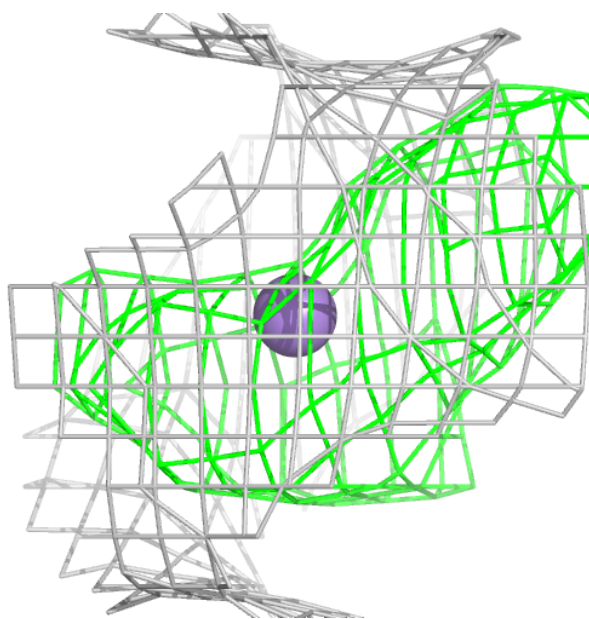






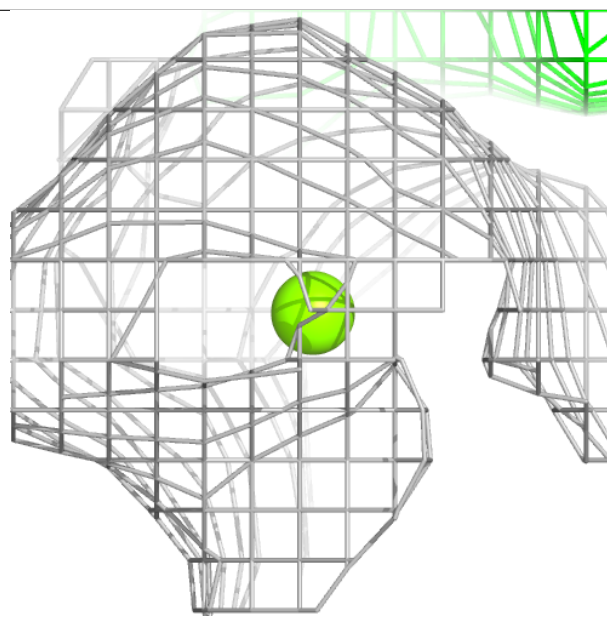
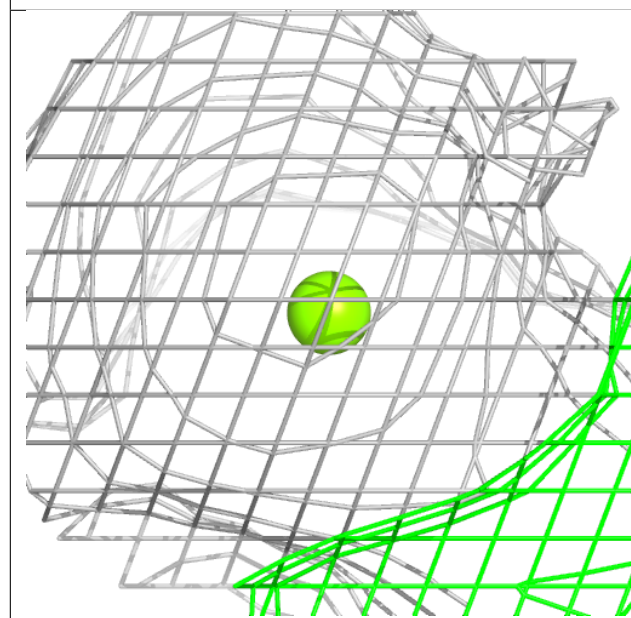
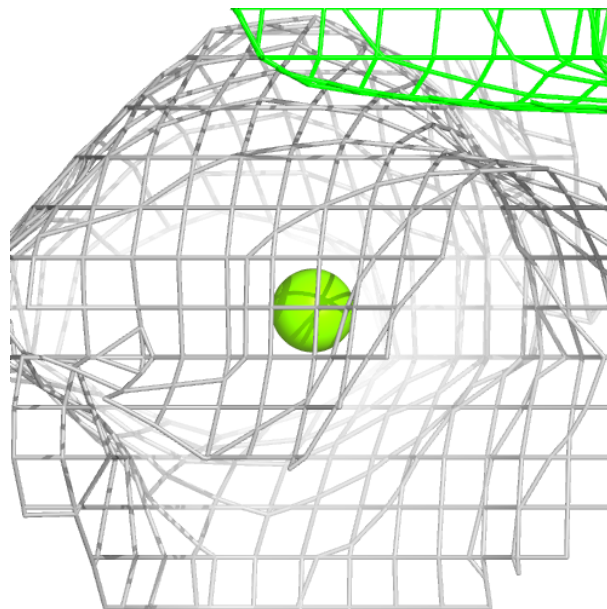
Electron density around MN D 1108:

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



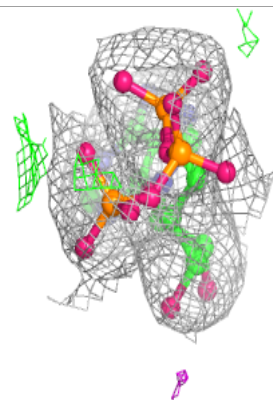
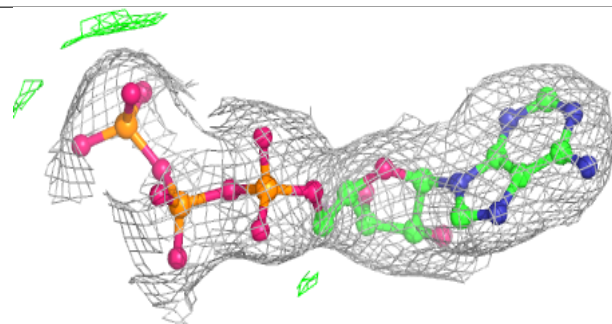
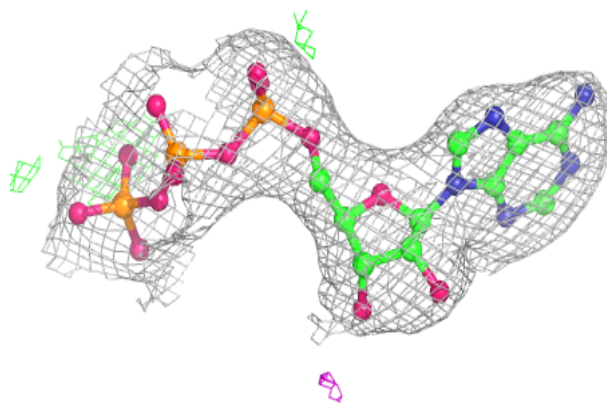
Electron density around MG A 403:

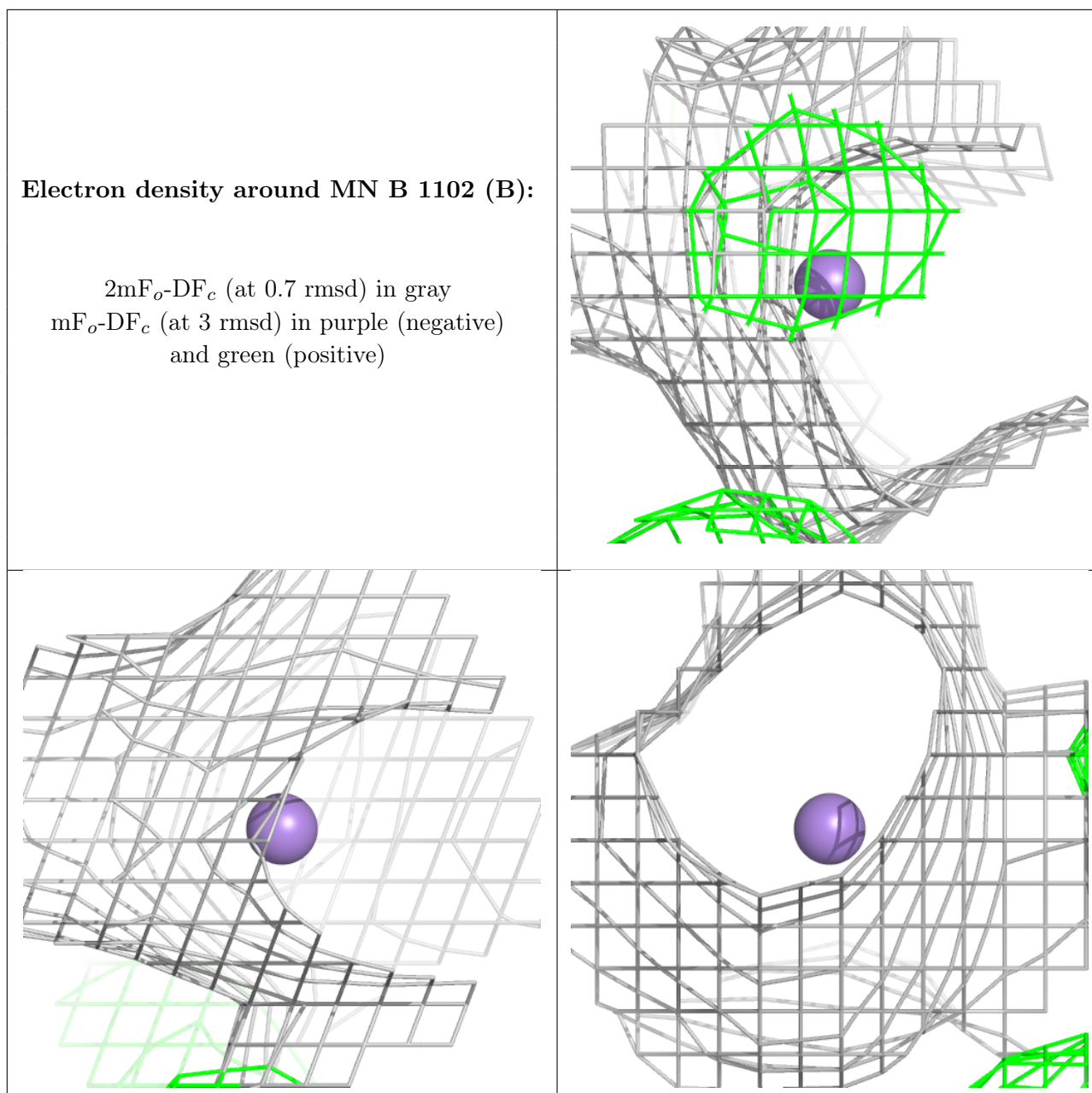
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

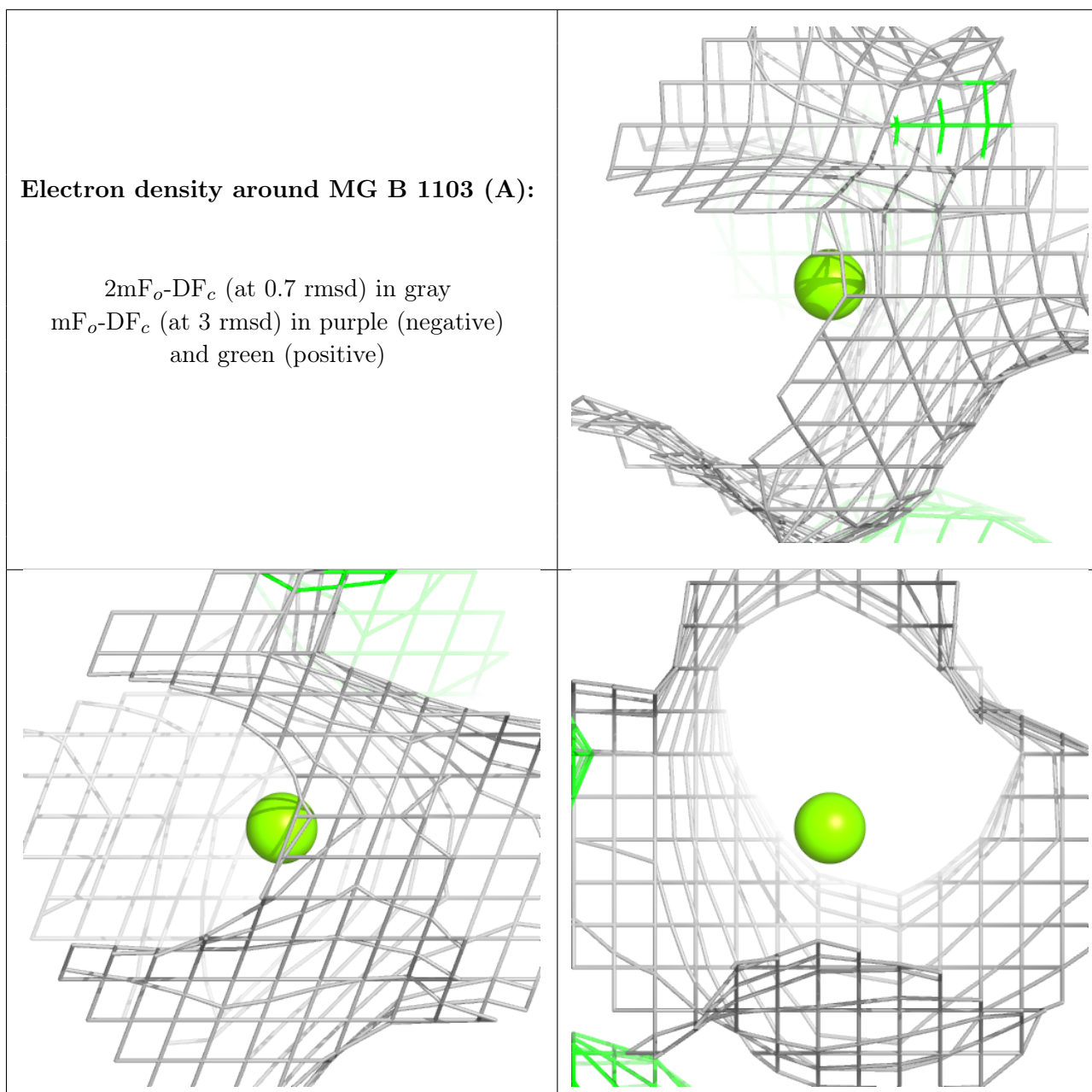


Electron density around ATP A 402:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.